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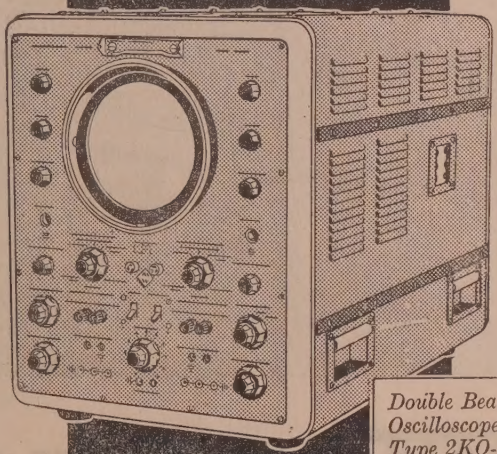

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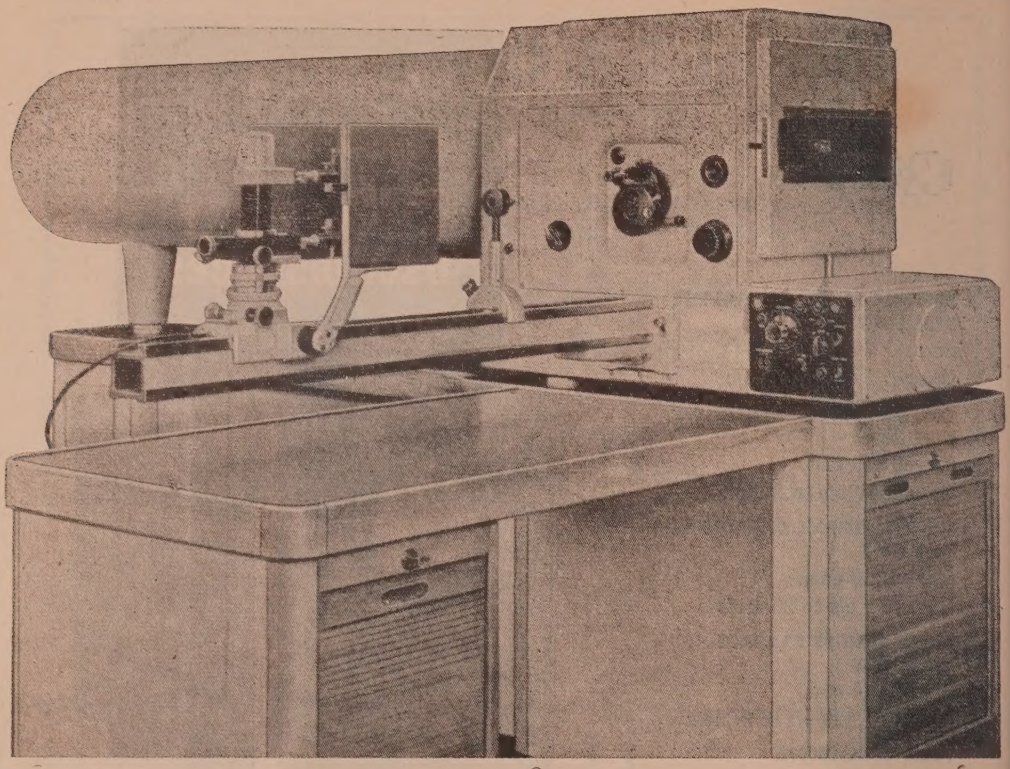

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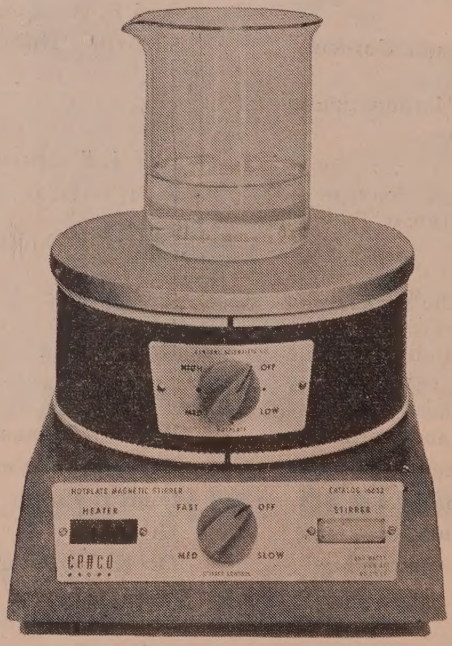

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11

A MICROWAVE ANALOGUE FOR X-RAY DIFFRACTION PART I. EFFECT OF THE CRYSTALLITE SIZE

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(*Received, January* 27, 1960)

ABSTRACT. Diffraction of X-rays by a crystal is analogous to that of microwaves by a three dimensional array of scatterers when the distance of one scatterer from another is of the same order of magnitude as the wave length of the microwaves. Thus all phenomena connected with the diffraction of X-rays by crystals are expected to be obtained due to the scattering of microwaves by a three dimensional arrangement of scatterers. To verify this, metallic scatterers in the form of small cylinders have been arranged to form the model of a crystal having tetragonal lattice parameter of $a = 3.2$ cm. and $c = 4.8$ cm. A lattice of 900 such unit cells have been irradiated by microwaves of wavelength 3.2 cms. Bragg's law has been found to be valid for the (100) and (110) planes of this crystal model. The intensity distribution curves around these two reflection maxima have been studied for 10, 7 and 4 planes in the b-direction. The half intensity widths have been compared with the formula due to Scherrer. Scherrer formula has been found to agree fairly well with experimental data.

INTRODUCTION

As is well known, all the phenomena concerning diffraction of X-rays by crystals have been explained on the basis of extremely short wavelength electromagnetic waves being scattered by atoms placed at the lattice points of a three dimensional periodic structure. The scattered electromagnetic waves interfere with each other and in the directions they reinforce each other there is obtained a diffraction maximum. The pattern of the diffraction maxima depends on the arrangement of the atoms in the crystal. Thus a study of the diffraction pattern of a crystal reveals the arrangement of atoms in it.

If a lattice is constructed with metal or dielectric scatterers at the lattice points, the lattice constants being of the order of centimeters, its behaviour towards centimetre wavelength microwaves should be exactly similar to that of a crystal to *X*-rays. Recently Allen (1955) described the verification of Bragg's law for 12-cm wave length microwaves and a model cubic structure of lattice constant 16 cm having metal discs mounted on wooden rods. The model was eight planes long, 4 planes high and two planes deep and so consisted of sixty-four unit cells only. Allen obtained diffraction maxima in the first order as well as in the second order for the (100) planes only. Since this is the first experiment of its kind, it

has been considered worth while to repeat the experiment for another crystallographic system, viz the tetragonal class with larger number of unit cells so that a crystal could be simulated more realistically. It has also been decided to study the effect of the crystal size on the width of the intensity distribution curves.

EXPERIMENTAL

A lattice containing nine hundred unit cells has been constructed with brass scatterers at the lattice points. The brass scatterers were cylinders having 1 cm diameter and 0.5 cm height and provided with a small hole in the middle for passing plastic threads through them. The plastic threads without scatterers were tested for their scattering power and were observed to have none or at least very little. This lattice was supported in a wooden structure provided with arrangements for quick rearrangement of the scatterers. The lattice constants in this case were $a = 3.2$ cm, $b = 3.2$ cm and $c = 4.8$ cm.

The lattice was irradiated by a microwave horn and the diffraction pattern about the lattice was measured by another microwave horn. Both these horns could be rotated about a common vertical axis of the lattice. The microwave signal was generated by a klystron (723A/B) and was fed to the radiating horn. The second microwave horn, acting as a receiving antenna, picked up the diffracted signal and fed into a crystal detector. The klystron was square-wave modulated and the video square wave at the output of the detector was measured by an amplifier. The diffraction pattern was obtained by recording the putput of the amplifier at various settings of the receiving horn for a pre-determined position of the transmitting horn. The scattering due to the wooden frame and the walls etc. of the room was first of all studied to determine the zero level of the signal received by the detector. This was made very low compared to the signal from the three dimensional array. The polar diagramme of the radiating horn was studied to find out the effect of instrumental broadening on the intensity distribution curves.

RESULTS AND DISCUSSIONS

The incident beam of microwaves was normal to the (001) direction and readings were taken only for the (100) and (110) planes. A diffraction maximum was obtained for both the incident as well as the diffracted beams making an angle of 30° with the planes parallel to the X-axis. This corresponds to the Bragg angle for the (100) plane of the lattice under investigation. Similarly, a diffraction maximum was again observed at 44° corresponding to the Bragg angle for the (110) planes. Thus Bragg law was found to be satisfied at least in these two cases.

Next the effect of particle size was investigated. The intensity *vs* angle curves in the vicinity of the 44° and 30° scattering maxima for 10, 7 and 4 planes in the b-direction were drawn and their half intensity angular widths were

determined after eliminating the instrumental broadening. The results are shown in Table I and in Figs. 1 and 2.

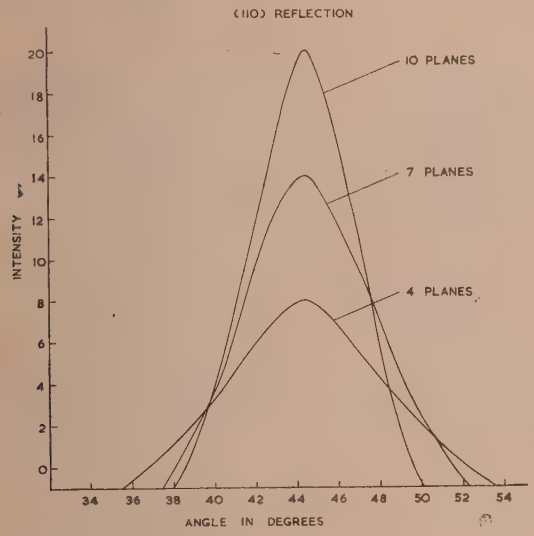

Fig. 1

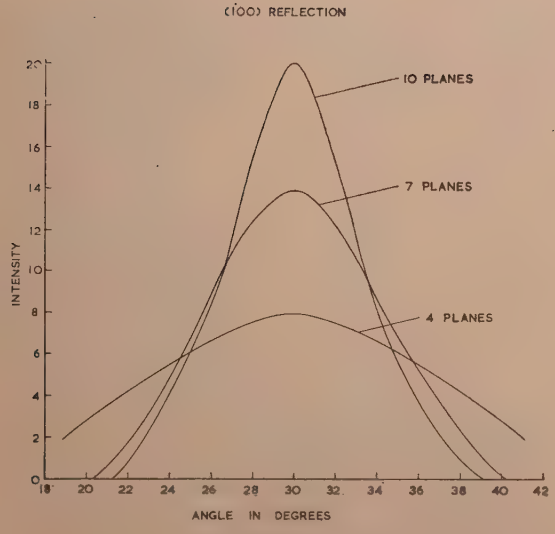

Fig. 2

The measured half intensity widths have been compared with those calculated from the well-known Scherrer formula (1918). While calculating the half intensity width

$$\beta = \frac{\lambda}{t \cos \theta}$$

where λ is the wavelength, θ the Bragg angle and t the crystallite size, t has been taken to be the thickness of the crystallite in the (hkl) direction. It is observed that the measured half intensity widths agree rather fairly well with the Scherrer formula. It is to be noted that all the planes normal to the (110) direction did not have the same number of scatterers in them. The end planes possessed very few scatterers. It is clear that it is necessary to have the intensity curves for the planes free from overlap from scatterings due to other planes. To achieve this, the lattice dimensions have been so taken that only two Bragg reflections, namely, at 30° and 44°30′ are possible for the given setting of the crystal model. Even then there has been certain overlap between these scatterings due to the two planes. The intensity distribution curves shown in figures 1 and 2 have been drawn after eliminating the effects due to such overlap. It must be noted that in calculating the half intensity widths the measurements of the parameters involved have been fairly accurate. The close agreement of the measured half intensity widths with Scherrer's formula is rather interesting.

ACKNOWLEDGMENT

Thanks are due to Dr. H. Rakshit and to Dr. K. Banerjee for their kind interest in this work.

TABLE I

Plane (hkl)	Bragg angle θ degrees	Thickness of crystal in the (hkl) direction t cms.	Half intensity angular width calculated from Scherrer formula	Observed half intensity width β in degrees
		32.0	6°36′	7°
100	30°	22.4	9°48′	11°
		12.8	16°32′	17°
		44.8	5°44′	6°
110	44°30′	39.1	6°34′	7°
		34.5	7°28′	8°

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12

OSCILLATIONS OF ROTATING COSMICAL BODIES IN THE PRESENCE OF MAGNETIC FIELD

J. N. TANDON

Indian National Committee for the IGY, National Physical Laboratory, Delhi

(*Received, February* 6, 1960)

ABSTRACT. The effect of rotation on the radial pulsations of cosmical fluid masses with special reference to spherical mass (magnetic variables) and cylindrical mass (spiral arm, solar-ion stream) has been investigated when the fluids are having volume electric currents. Two models of currents system are considered for cylindrical mass, viz., circular currents and line currents. It is found that for radial pulsations, rotation in general, helps in the dynamical stability of the cosmical bodies.

1. INTRODUCTION

Talwar and Tandon (1956) have earlier obtained an expression for the frequency of radial pulsations of spherical masses in the presence of megnetic field (magnetic variable stars). The magnetic field was assumed to be axially symmetric and derivable from volume currents flowing in the interior of the star. They also obtained an upper limit for the magnetic field above which the star will become dynamically unstable provided $\Gamma > 4/3$ where Γ is the ratio of the two specific heats. Similar problem for radial pulsations of the infinitely long cylinder (spiral arm solar-ion streams etc.) having volume currents has also been investigated by Tandon and Talwar (1957). Two special cases, (1) circular currents and (2) line currents are investigated. It is found that the cylinder remains dynamically stable for both the models.

In this paper we have investigated the effect of rotation on the frequency of pulsations of the cosmical masses having volume currents. §2 deals with the radial pulsations of rotating spherical mass and is of great significance for magnetic variables. Ledoux (1945) has treated the similar problems for non-magnetic stars and has obtained the expression for frequency of radial pulsations. Our expression is similar to one obtained by Ledoux except that an additional term $\int \mathbf{r} \cdot (\mathbf{J} \times \mathbf{H})\, d\tau$ along with gravitational energy term Ω has been obtained. It is also shown that rotation helps in the dynamical stability of the star provided $\frac{4}{3} < \Gamma < \frac{5}{3}$. In §3 we have considered the effects of the rotation on the radial pulsations of cylindrical fluid masses. The two special cases of the volume currents, viz., circular and line currents have been re-investigated. It is found that rotation helps in the dynamical stability of the cylinder also.

2. PULSATIONS OF ROTATING SPHERE WITH VOLUME CURRENTS

The equation of motion of a uniformly rotating fluid mass having an internal magnetic field arising from the volume currents can be written as

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho}\,\text{grad}\,p - \text{grad}\,V + \frac{1}{\rho}(\mathbf{J}\times\mathbf{H})$$

$$-\mathbf{w}\times(\mathbf{w}\times\mathbf{r}) - 2(\mathbf{w}\times\mathbf{u}) - \left(\frac{d\mathbf{w}}{dt}\times\mathbf{r}\right) \quad \ldots \quad (1)$$

where ρ denotes the fluid density, V the gravitational potential, p the pressure and $\mathbf{w}$ the angular velocity at any point. The magnetic field $\mathbf{H}$ and the current density $\mathbf{j}$ satisfy the following relation inside

$$\text{curl}\,\mathbf{H} = 4\pi\mathbf{J} \quad \ldots \quad (2)$$

$$\text{div}\,\mathbf{H} = 0 \quad \ldots \quad (3)$$

and the field outside is continuous at the boundary.

Assuming axial symmetry, $\mathbf{u}$ the fluid velocity vector will be in the meridian plane and the last two terms on the right hand side of eqn.(1) are the only vector in this equation which are normal to this plane*. Thus we should have

$$2(\mathbf{w}\times\mathbf{u}) + \left(\frac{d\mathbf{w}}{dt}\times\mathbf{r}\right) = 0 \quad \ldots \quad (4)$$

and

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho}\,\text{grad}\,p - \text{grad}\,V + \frac{1}{\rho}(\mathbf{J}\times\mathbf{H}) - \mathbf{w}\times(\mathbf{w}\times\mathbf{r}) \quad \ldots \quad (5)$$

We multiply equation (5) scalarly on a vector $\mathbf{r}$ and integrate over the entire mass of the configuration. The left hand side of the equation becomes

$$\int^{M} \mathbf{r}\cdot\frac{d\mathbf{u}}{dt}\,dm = \int^{M} \mathbf{r}\cdot\frac{d^2r}{dt^2}\,dm = \frac{1}{2}\frac{d^2}{dt^2}\int^{M} r^2 dm - \int^{M} |u|^2 dm \quad \ldots \quad (6)$$

where $dm = \rho d\tau (= \rho dx_1\,dx_2\,dx_3)$

and the integration is effected over the entire mass, M, of the configuration.

* It may be noted here that we are restricting ourselves to a case when the electromagnetic force $j \times H$ also lies only in the meridian plane.

Letting

$$I = \int^{M} r^2 dm$$

and

$$T = \frac{1}{2} \int^{M} |u|^2 dm$$

denote the movement of inertia and kinetic energy of mass motion respectively, we have

$$\frac{1}{2}\frac{d^2 I}{dt^2} - 2T = -\int_V \mathbf{r} \cdot \text{grad}\, p\, d\tau + \int^{M} \frac{1}{\rho}\, r.(\mathbf{j}\times\mathbf{H}) dm$$

$$- \int^{M} \mathbf{r} \cdot (\text{grad V}) dm - \int^{M} \mathbf{r} \cdot \{\mathbf{w}\times(\mathbf{w}\times\mathbf{r})\} dm \quad \ldots \quad (7)$$

The third integral on the right hand side of this equation represents the gravitational potential energy Ω of the configuration. Now

$$\int_V \mathbf{r} \cdot \text{grad}\, p\, d\tau = \int_S p\, \mathbf{r}.d\mathbf{S} - \int_V p\, div\, \mathbf{r}\, d\tau = -3\int_V p\, d\tau \quad \ldots \quad (8)$$

since the gas pressure vanishes at the boundary of the surface. Thus we should have

$$\int_V \mathbf{r} \cdot \text{grad}\, p\, d\tau = -3(\Gamma - 1)U \quad \ldots \quad (9)$$

where U is the internal energy of the system. Now, since $\mathbf{r}.\ \mathbf{w} = 0$, the last integral on the right hand side of equation (8) can be written as

$$\int^{M} \mathbf{r} \cdot \{\mathbf{w}\times(\mathbf{w}\times\mathbf{r})\} dm = -\int^{M} w^2(x^2+y^2) dm$$

$$= -\int^{m} w dm \quad \ldots \quad (10)$$

$$= -\, wW$$

where W is the total angular momentum. Further, putting

$$\int^{M} \frac{1}{\rho}\, \mathbf{r} \cdot (\mathbf{j}\times\mathbf{H}) dm = E \quad \ldots \quad (11)$$

the electromagnetic energy of the fluid, and substituting the values of various integrals in equation (8) we find

$$\frac{1}{2}\frac{d^2 I}{dt^2} = 2T + 3(\Gamma - 1)u + \Omega + E + wW \quad \ldots \quad (12)$$

This is the Virial theorem for a system of rotating fluid subjected to electromagnetic field. We shall now apply this equation to the adiabatic pulsations of a rotating fluid in which there are body currents. In analysing this problem we shall adopt the Lagrangian mode of description and follow each element of mass, dm, as it moves.

Considering periodic oscillations with angular frequency we shall let $\delta\mathbf{r}e^{i\sigma t}$ denote the displacement of an element of mass dm, from its equilibrium position r_0. Similarly, we shall denote by $\delta pe^{i\sigma t}$, $\delta\rho e^{i\sigma t}$, $\delta\mathbf{H}e^{i\sigma t}$, $\delta\mathbf{j}e^{i\sigma t}$ and $\delta\mathbf{w}e^{i\sigma t}$ the corresponding changes in the other physical variables as we follow the element, dm, during its motion. The assumption that oscillations take place adiabatically requires that the changes in pressure and density, as we follow the motion, should satisfy the relation

$$\delta p = \Gamma \frac{\delta\rho}{\rho} p \qquad \ldots \quad (13)$$

where Γ is the ratio of the specific heats (assumed to be constant in space and time) while the equation of continuity

$$\frac{\partial\rho}{\partial t} + \rho \text{ div } \mathbf{u} = 0$$

requires that

$$\frac{\delta\rho}{\rho} = - \text{ div } \delta\mathbf{r} \qquad \ldots \quad (14)$$

Returning to equation (4) and assuming Z-axis as the axis of rotation we can write it in cylindrical coordinate system (ω, θ, z) as follows

$$2w \frac{\partial\omega}{\partial t} + \omega \frac{\partial\omega}{\partial t} = 0 \qquad \ldots \quad (15)$$

Upon integration this leads to the relation

$$w\omega^2 = \text{constant} \qquad \ldots \quad (16)$$

which can also be expressed in cartesians as follows

$$w(x^2+y^2) = \text{constant} \qquad \ldots \quad (17)$$

Equation (4) simply expresses the conservation of angular momentum w.

Letting $\delta Ie^{i\sigma t}$, $\delta\Omega e^{i\sigma t}$, $\delta ue^{i\sigma t}$, $\delta Ee^{i\sigma t}$ and $\delta(wW)e^{i\sigma t}$ denote the changes in I, Ω U, E and wW respectively we can write equation (12) as

$$-\tfrac{1}{2}\sigma^2\delta I = 3(\Gamma-1)\delta u + \delta\Omega + \delta E + \delta(wW), \qquad \ldots \quad (18)$$

Since to the first order in the displacement, the terms involved in T do not make any significant contribution.

Now

$$\delta I = 2\int^{M} \mathbf{r} \,.\, \delta\mathbf{r} dm \qquad \ldots \quad (19)$$

$$3(\Gamma - 1)\delta U = 3\int^{M} \delta(p/\rho) dm$$

$$= 3\int^{M} \left(\frac{\delta p}{\rho} - \frac{p\delta\rho}{\rho^2} \right) dm$$

$$3(\Gamma - 1)\int^{M} \frac{p}{\rho}\frac{\delta\rho}{\rho} dm$$

$$= -3(\Gamma - 1)\int_{V} p \text{ div } \delta\mathbf{r}\, d\tau$$

$$= -3(\Gamma-1)\left[\int_{S} p\mathbf{r} \,.\, d\mathbf{s} - \int_{V} \delta\mathbf{r} \,.\, \text{grad } p\, d\tau\right]$$

$$= 3(\Gamma-1)\int_{V} \delta\mathbf{r} \,.\, \text{grad } p\, d\tau \qquad \ldots \quad (20)$$

In obtaining equation (20) we have made use of the equations (13) and (14) and of the fact that the fluid pressure vanishes on the bounding surface. Further for the equilibrium configuration equation (5) gives

$$\text{grad } p = -\rho \text{ grad } V + (\mathbf{J}\times\mathbf{H}) - \rho\mathbf{w}\times(\mathbf{w}\times\mathbf{r}) \qquad \ldots \quad (21)$$

Therefore

$$3(\Gamma-1)\delta U = 3(\Gamma-1)\int_{V} \delta\mathbf{r} \,.\, \text{grad } p d\tau$$

$$= 3(\Gamma-1)\left[-\int^{M} \delta\mathbf{r} \,.\, \text{grad } V\, dm\right.$$

$$+\int_{V} \delta r \,.\, (\mathbf{J}\times\mathbf{H}) d\tau \qquad \ldots \quad (22)$$

$$\left.-\int^{M} \delta\mathbf{r} \,.\, \{\mathbf{w}\times(\mathbf{w}\times\mathbf{r})\} dm\right]$$

Further, we have

$$\delta\Omega = -\int^{M} \delta\mathbf{r} \,.\, \text{grad } V\, dm \qquad \ldots \quad (23)$$

But

$$\delta E = \delta \int^{M} \frac{1}{\rho}\, \mathbf{r} \,.\, (\mathbf{J}\times\mathbf{H}) dm$$

$$= \int^{M} \left[\left\{ \frac{\delta \mathbf{r}}{\rho} - \frac{\delta\rho}{\rho^2}\, \mathbf{r} \right\} (\mathbf{J}\times\mathbf{H}) \right.$$

$$\left. + \mathbf{r} \,.\, \{(\delta\mathbf{j}\times\mathbf{H}) + (\mathbf{J}\times\delta\mathbf{H})\} \right] dm$$

$$= \int_{V} [\{\delta\mathbf{r} + (\text{div } \delta\mathbf{r}) \,.\, \mathbf{r}\}(\mathbf{J}\times\mathbf{H}) \qquad \ldots \quad (24)$$

$$+ \mathbf{r} \,.\, \{(\delta\mathbf{J}\times\mathbf{H}) + (\mathbf{J} + \delta\mathbf{H})\}] d\tau$$

and since the total angular momentum is preserved during pulsations, we have

$$\delta(wW) = W\delta w \qquad \ldots \quad (25)$$

Substituting equations (19) to (25) in equation (18) we get

$$-\sigma^2 \int^{M} \mathbf{r} \,.\, \delta\mathbf{r}\, dm = -(3\Gamma - 4) \int^{M} \delta\mathbf{r} \,.\, \text{grad } V dm$$

$$+ (3\Gamma - 2) \int_{V} \delta\mathbf{r} \,.\, (\mathbf{J}\times\mathbf{H}) d\tau$$

$$+ \int_{V} (\text{div } \delta\mathbf{r})\, \mathbf{r} \,.\, (\mathbf{J}\times\mathbf{H}) d\tau \qquad \ldots \quad (26)$$

$$+ \int_{V} \mathbf{r} \,.\, [(\delta\mathbf{J}\times\mathbf{H}) + (\mathbf{j}\times\delta\mathbf{H})] d\tau$$

$$- 3(\Gamma - 1) \int^{M} \delta\, \mathbf{r} \,.\, \{\mathbf{w}\times(\dot{\mathbf{w}}\times\mathbf{r})\} dm$$

$$+ W\ \delta w$$

This is the required integral formula for σ^2. The change δH following the motion is given by (Chandrasekhar and Fermi, 1953).

$$\delta\mathbf{H} = \text{curl } (\delta\mathbf{r}\times\mathbf{H}) + (\delta\mathbf{r} \,.\, \text{grad})\, \mathbf{H}$$

while $\delta\mathbf{j}$ will be evaluated by substituting the value of this in equation (2) remembering that the independent variable is r_0 and not r while following the motion.

To obtain the approximate relation for the frequency of pulsations we put,

$$\delta\mathbf{r} = \xi\mathbf{r} \qquad \ldots \quad (28)$$

where ξ is constant in space. Thus it can readily be seen that

$$\left.\begin{aligned}\delta\mathbf{H} &= -2\xi\mathbf{H}\\ \delta\mathbf{j} &= -3\xi\,\mathbf{j}\\ \delta\mathbf{w} &= -2\xi\mathbf{w}\end{aligned}\right\} \quad \ldots \quad (29)$$

and

$$\int^{M} \delta\mathbf{r}\,.\,\{\mathbf{w}\times(\mathbf{w}\times\mathbf{r})\}dm = -\xi\; w\; W$$

Substituting equations (28) and (29) in equation (27) we obtain after some reduction

$$\sigma^2 \int^{M} r^2 dm = -(3\Gamma-4)[E+\Omega]+(5-3\Gamma)wW$$

or

$$\sigma^2 = -(3\Gamma-4)\,\frac{E+\Omega}{I} + (5-3\Gamma)\,\frac{wW}{I} \quad \ldots \quad (30)$$

It is evident from equation (30) that rotation like gravitation helps in the dynamical stability of the sphere provided $\frac{4}{3} < \Gamma < \frac{5}{3}$. Also there exists an upper limit for the magnetic field set by the following equation, viz.,

$$E = |\,\Omega\,| - \frac{3\Gamma-5}{3\Gamma-4}\; wW \quad \ldots \quad (31)$$

3. RADIAL PULSATIONS OF A ROTATING CYLINDER WITH VOLUME CURRENTS

Let us now consider an infinitely long cylinder, rotating with a constant angular velocity $\mathbf{w}$ in which the currents are flowing. The equation of motion for the radial pulsation of such a configuration assuming axial symmetry can be written as follows*

$$\frac{du_w}{dt} = -\frac{1}{\rho}\,\frac{\partial p}{\partial \omega} - \frac{2Gm(\omega)}{\omega} + \frac{1}{\rho}\,(\mathbf{j}\times\mathbf{H})_{radial} - \{\mathbf{w}\times(\mathbf{w}\times\omega)\}_{radial} \quad \ldots \quad (32)$$

and

$$2(\mathbf{w}\times\mathbf{u}) + \left(\frac{d\mathbf{w}}{dt}\times\omega\right) = 0 \quad \ldots \quad (33)$$

Here $m(\omega)$ is the mass of the unit length of the cylinder interior to ω. Equation (33) with Z-axis of the cylindrical coordinate system (ω, θ, z) as the axis of the rotation can be written in the form (after integration)

$$w\omega^2 = \text{constant} \quad \ldots \quad (34)$$

* Here we assume that $j\times\mathbf{H}$ has only radial component,

This equation simply expresses the conservation of angular momentum. Multiplying equation (32) by ω and integrating over the entire mass of unit cylinder and proceeding exactly as in § 2, we find

$$\int^{M} \omega \frac{du_w}{dt} = \frac{1}{2}\frac{d^2}{dt^2}\int^{M} \omega^2 dm - 2T \qquad \ldots (35)$$

where M is the mass of the unit cylinder and T is the kinetic energy of the mass motion. Also,

$$\int^{M} \frac{\omega}{\rho}\frac{\partial p}{\partial \omega}\, dm = -2\int_{V} p d\tau = -2(\Gamma - 1)U \qquad \ldots (36)$$

since div $\omega = 2$, for a 2 dimensional case and U is the internal energy per unit length of the comfiguration. For a homogeneous fluid mass we further have

$$\int^{M} \omega \,.\, \frac{2Gm}{\omega}\, dm = GM^2 \qquad \ldots (37)$$

$$\int^{M} \frac{1}{\rho}\, \omega \,.\, (\mathbf{J}\times\mathbf{H}) dm = E \qquad \ldots (38)$$

and

$$\int^{M} \omega \,.\, \{\mathbf{w}\times(\mathbf{w}\times\omega)\} dm = -\int^{W} w dW = -wW \qquad \ldots (39)$$

where $dW = w\omega^2$ and m is the angular momentum per unit length of the cylinder. Hence the Virial theorem for the study of radial pulsations of an rotating infinite cylinder having volume currents will be

$$\frac{1}{2}\frac{d^2}{dt^2}\int^{M} \omega^2 dm = 2T + 2(\Gamma - 1)U - GM^2 + E + wW \qquad \ldots (40)$$

To study the radial pulsations we adopt as before Lagrangian mode of description. Now consider periodic pulsations with the frequency σ and let $\delta\omega e^{i\sigma t}$ denote the displacement of an element of mass, dm, from its equilibrium configuration, ω_0. Similarly, denote the corresponding changes in other physical variables by $\delta p e^{i\sigma t}$ etc. Further, the change in the pressure δp for adiabatic pulsations and the equation of continuity are represented by equations (13) and (14) respectively.

Letting $\delta u e^{i\sigma t}$, $\delta m e^{i\sigma t}$ and $\delta(wW)e^{i\sigma t}$ denote the changes in quantities U, E and wW we have from the Virial theorem

$$-\sigma^2 \int^{M} \omega \delta\omega dm = 2(\Gamma - 1)\delta U + \delta E + \delta(wW) \qquad \ldots (41)$$

Since GM^2 is constant and to the first order in the displacement, the terms in T will not make any contribution. Further,

$$2(\Gamma-1)\delta U = 2(\Gamma-1)\int_V \delta\omega \frac{\partial p}{\partial \omega}\, d\tau$$

since the pressure vanishes at the bounding surface. Now for the equilibrium configuration

$$\frac{\partial p}{\partial \omega} = -\frac{2Gm}{\omega}\rho + (\mathbf{J}\times\mathbf{H})_{radial} - \rho\{\mathbf{w}\times(\mathbf{w}\times\omega)\}_{radial}$$

Multiplying this equation by $\delta\omega$ and putting

$$\delta\omega = \xi\omega \qquad \ldots \quad (42)$$

we find

$$2(\Gamma-1)\delta U = 2(\Gamma-1)[-\int^M \xi Gm\, dm + \int_V \xi\omega\,.\,(\mathbf{J}\times\mathbf{H})d\tau + \int^W \xi w dW] \qquad \ldots \quad (43)$$

Further

$$\delta E = \int_V \{\xi + \mathrm{div}(\xi\omega)\}\{\omega\,.\,(\mathbf{J}\times\mathbf{H})\}d\tau + \int_V \omega\,.\,[(\delta\mathbf{j}\times\mathbf{H}) + (\mathbf{J}\times\delta\mathbf{H})]d\tau \qquad \ldots \quad (44)$$

and

$$\delta(wW) = W\,\delta w \qquad \ldots \quad (45)$$

since the angular momentum is constant. Now from equation (34) we get

$$\delta w = -2\xi W$$

Therefore

$$\delta(wW) = -2\xi w W$$

Hence equation (41) with the help of equations (43) to (46) reduces to

$$-\sigma^2 \int^M \xi\omega^2 dm = -2(\Gamma-1)\Big[\int^M \xi 2Gm dm - \int_V \xi\omega\,.\,(\mathbf{J}\times\mathbf{H})d\tau$$

$$- \int^{w} w\xi dm \Big] + \int_{V} [\xi + \mathrm{div}(\xi\omega)][\omega \,.\, (\mathbf{J} \times \mathbf{H})]d\tau$$

$$+ \int_{V} \omega \,.\, [(\delta\mathbf{j} \times \mathbf{H}) + (\mathbf{J} \times \delta\mathbf{H})]d\tau - 2\xi wW \quad \ldots \quad (47)$$

This is the required integral formula for the frequency of radial pulsations of rotating infinitely long cylinder for all currents distribution having axial symmetry. The changes $\delta\mathbf{H}$ in the magnetic field and $\delta\mathbf{j}$ in the current density can easily be evaluated with the help of equations (27) and (2).

Let us now obtain the approximate expression for the frequency of pulsation for two special cases of magnetic fields, viz.. poloidal and toroidal. Auluck and Kothari (1957) have discussed these two systems of fields in detail. Let us make use of the usual assumption made in the theory of adiabatic pulsations of stars, viz.,

$$\xi = \text{constant in space.} \quad \ldots \quad (48)$$

Case (i) The magnetic field is poloidal.

This poloidal magnetic field is derived from circular currents of the form

$$\mathbf{j} = \left\{ 0, -\frac{k\omega}{4\pi}, 0 \right\} \quad \ldots \quad (49)$$

such that

$$\mathbf{H} = \left\{ 0, 0, \frac{k}{2}(\omega^2 - R^2) \right\} \quad \ldots \quad (50)$$

where k is constant and R is the radius of the cylinder. For such a configuration, it was shown earlier by Tandon and Talwar (1957) that

$$\delta\mathbf{H} = -2\xi\mathbf{H}$$

and

$$\delta\mathbf{j} = -3\xi\mathbf{j} \quad \ldots \quad (51)$$

The equation for the frequency of radial pulsations will then be

$$\sigma^2 \int^{M} \omega^2 dm = 2(\Gamma - 1)GM^2 - 2(\Gamma - 2) \int_{V} \omega,(\mathbf{J} \times \mathbf{H})d\tau$$

$$- 2(\Gamma - 2)wW. \quad \ldots \quad (52)$$

or using the abbreviation

$$E' = \int_{V} \frac{H^2}{8\pi} d\tau \quad \ldots \quad (53)$$

we get

$$\sigma^2 \int^{M} \omega^2 dm = 2(\Gamma - 1)GM^2 + 2(2 - \Gamma)[2E' + wW] \quad \ldots \quad (54)$$

Thus, in the case of rotation the term $2E'$ of equation (25) of Tandon and Talwar has been replaced by $2E' + wW$. This clearly indicates that the rotation is similar to magnetic field and helps in the dynamical stability of the cylinder for radial pulsations in the presence of circular currents.

Case (ii)—The magnetic field is toroidal.

For this case we consider a system in which there are line currents of constant value such that

$$\mathbf{j} = \left(0, 0, \frac{k}{2\pi}\right) \quad \ldots \quad (55)$$

and hence

$$\mathbf{H} = (0, k\omega, 0) \quad \ldots \quad (56)$$

where k is a constant. The change in the magnetic field $\delta\mathbf{H}$ and the change in the current density $\delta\mathbf{j}$ will then be given by

$$\delta\mathbf{H} = -\xi\mathbf{H}$$

and $\quad \ldots \quad (57)$

$$\delta\mathbf{j} = -2\,\xi\,\mathbf{j}$$

The equation for the frequency of pulsations thus becomes

$$\sigma^2 \int^{M} \omega^2 dm = 2(\Gamma - 1)GM^2 - 2(\Gamma - 1)\int_V \omega \cdot (\mathbf{J} \times \mathbf{H}) d\tau + 2(\Gamma - 2)wW \quad \ldots \quad (58)$$

Further using the abbreviation represented by equation (53) we obtain

$$\sigma^2 \int^{M} \omega^2 dm = 2(\Gamma - 1)GM^2 + 8(\Gamma - 1)E' + 2(2 - \Gamma)wW \quad \ldots \quad (59)$$

This equation clearly indicates that the cylinder is stable for the radial pulsations in the presence of line currents as well.

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13

AN ARC TYPE WATER-COOLED ION SOURCE FOR POSITIVE IONS*

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ABSTRACT. An arc type water-cooled ion source for positive ions of simple construction and reliable operation is described in which the anode-filament assembly can be readily changed. The characteristic curves of the source are given. Operating at an arc current of 0.4 amp a total beam current of 500 micro-amperes is produced with a probe potential of about 3000 volts.

INTRODUCTION

A low voltage arc type ion source was installed in 1955 in connection with a 500 Kv Van de Graaff accelerator to provide positive ions for nuclear disintegration experiments. The ion source described here is the third one to be tried out. The first ion source was based on a design of Allen (1938).

The second ion source and the third, the present one, incorporated improvements and simplifications on the original design. Attempts have been made to incorporate desirable features found in previous designs of various types of ion sources (Crane, 1937; Timoshenko, 1938; Smith and Scott, 1939; Livingston, Holloway & Baker 1939; Getting, Fisk & Vogt; 1939, Finkelstein, 1940: Allison 1948, Swann and Swingle, 1952, Goodwin 1953 and Barnett, Steir and Evans, 1953), e.g., reliability, long filament life, easy accessibility of parts, etc. The source has been constructed of materials readily available in the laboratory.

DESCRIPTION

The source is pictorially represented in Fig. 1. The construction of the source can be understood from Fig. 2. The body of the source is made of brass. The filament-anode assembly is mounted on a single plate (A) which can be readily replaced with a similarly constructed assembly. *a*, *b* and *c* are machine screws which hold the filament and anode sassembly. They also serve as electric leads through the porcelain insulators, which are made vacuum tight by using lead gaskets. The hard glass envelope *D* confines the discharge, otherwise the arc spreads out and little current can be drawn by the probe voltage. During the experiment it was found that occasionally discharges would take place between

* Communicated by Dr. J. C. Kameshwar Rav.

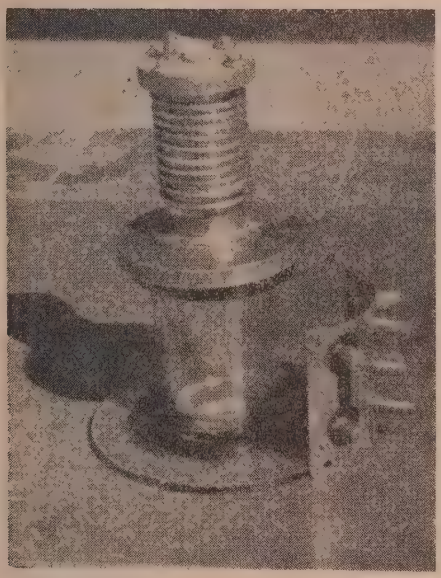

Fig. 1

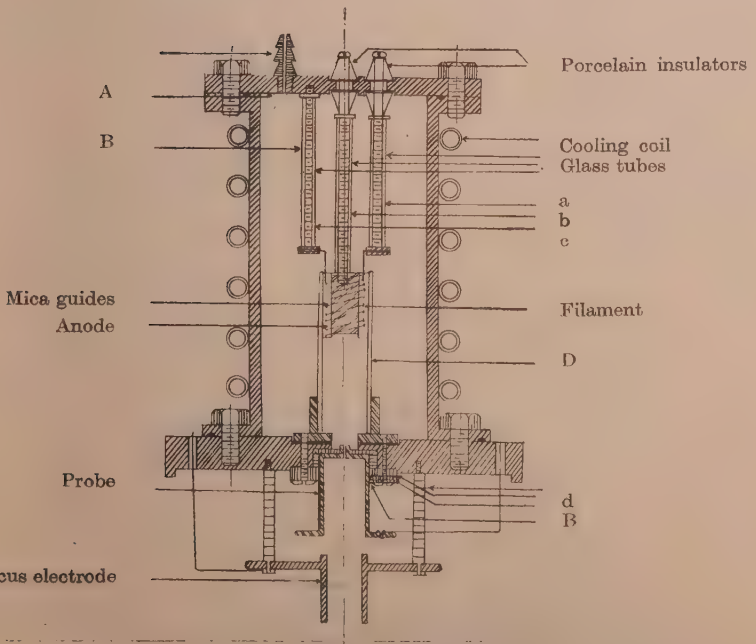
Porcelain insulators
A
B
Cooling coil
Glass tubes
a
b
c
Mica guides
Anode
Filament
D
Probe
d
B
Focus electrode

Fig. 2

the screws *a*, *b* and *c*; therefore, they have been covered with glass tubes to eliminate undesirable discharges. *B* is a Mycalex piece which holds the probe, which can be aligned by means of the screw *d*. The probe is made of steel and its front hole is drilled by No. 56 drill.

After considerable experience with tunsten-nickel combinations coated with alkaline earth oxides, we have decided on pure tungsten wire filaments. In the original design of Allen (1938) the distance between the anode and the filament was kept very small for easy starting of arc. Our experiments with close tungsten-nickel filaments coated with strontium and barium oxides have shown that although the arc would strike easily, sometimes the wire would break and would touch the anode thereby short-circuiting the power. Apart from this, unguided filaments are difficult to align with the result that the ion beam goes out of focus, as pointed out by Fulton and Gabrich (1952). In the new filaments, provision has been made to guide the helical form of the filament with three mica pieces. By using such guides the distance between the filament and the anode has been made uniformly as low as 3/32″. The filament is a helix of $\frac{1}{2}$ mm thick tungsten wire. It requires a current of 8–12 amps at about 8-12 volts. The striking voltage for the arc is about 250 volts, which is supplied from a 866A mercury vapour rectifier set.

The disappointing results with the oxide-coated tungsten-nickel filaments might be due to traces of oxygen present in hydrogen or vacuum system or due to non-trapping of organic vapours. However, pure tungsten filaments seem to be satisfactory except for heavy current consumption.

PERFORMANCE

The accelerator is operated with the ion source at ground potential, the accelerating tube being separate from the Van de Graaff generator. The usual electrical operating conditions of the ion source are given in Table I.

TABLE I

1.	Arc current	400 mA.
2.	Starting voltage for arc.	250 volts
3.	Voltage drop; anode to filament	88 volts
4.	Filament current	11 amps
5.	Filament voltage	9.5 volts
6.	Probe voltage	3.2 Kv
7.	Beam current	500 Micro-amp
8.	Focus voltage*	10.4 KV

* Applied while working the accelerator.

The curves of Fig. 3 show the beam current put out by the arc, and the current to the probe face, as a function of the probe voltage at various arc currents. The beam current is the current at the first electrode of the accelerating tube, next to the focus electrode (not shown here). There was no focussing voltage across the first gap during these measurements and the arc was operating on hydrogen gas.

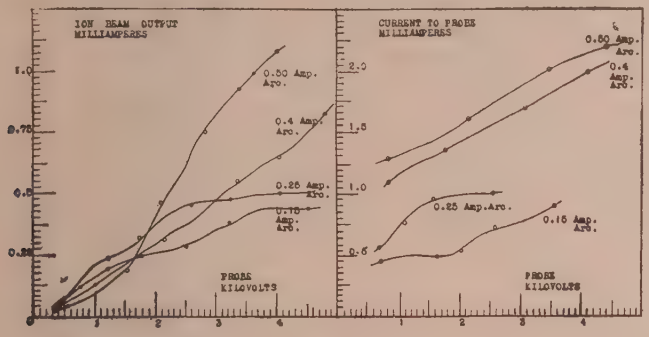

Fig. 3

Rough studies were made of the rate of consumption of the gas and the pressure when it was operating. The practice that has been followed is to adjust the leak till the pressure in the ion source rises to 1.5×10^{-3} mm of Hg, when measured with a gauge. The rate of consumption of the gas is then about 25 c.c. at atmospheric pressure per hour. The pumping speed on our accelerator as given by the manufacturers of the pumps and estimated from pump orifice dimensions is 40 litres per second.

We have two duplicate assemblies of the filaments made on another arc port plate. In order to change the filament assemblies, the diffusion pump is allowed to cool. With the fore pump in operation the entire plate is removed and the new plate inserted and tightened. The whole operation takes less than two minutes and the pressure rises a little through the probe canal. On the whole, the trouble due to any faults in the design has been negligible.

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14

THE EMISSION BAND SYSTEM OF IODINE IN THE BLUE VIOLET

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Plate I A & B

ABSTRACT. The D—B System of iodine molecule was found to be more extensively developed when the spectrum was excited in a condensed discharge from a high tension transformer. About 150 bands were newly classified as forming part of the previously known D—B system for which Waser and Wieland suggested the vibrational quantum formula.

INTRODUCTION

Recent investigations on the spectra of halogens by Haranath and Rao (1958) have led to the discovery of a number of discrete band systems in the spectral region $\lambda 2400$—$\lambda 1400$. Besides the above new results, a number of previously known systems in the visible and ultraviolet regions were also observed in the case of iodine, when the vapour was excited in a condensed discharge from a high tension transformer. The band system in the blue violet region $\lambda 4400$—$\lambda 4000$ was found to be more extensively developed than has been reported by previous workers. Only 40 bands obtained in fluorescence excitation by Elliot (1940) and about 80 in electrical excitation in the presence of argon by Venkateswarulu (1951) were known previously belonging to this system.

In the present work, the iodine spectrum excited at higher voltages of a condensed transformer revealed about 230 band heads some of which are clearly degraded towards longer wavelengths. This paper describes the results of the detailed investigations on the analysis of this band system attributed to neutral iodine molecule.

RESULTS

Details of the experimental technique employed for the excitation of the emission band spectrum of iodine in a condensed transformer discharge was already described by Haranath and Rao (1958). In the present work, the spectrum extending in the region $\lambda 4500$—$\lambda 3900$ was photographed mainly on Hilger 3 prism glass Littrow and Fuess spectrographs, the times of exposures being of 10 and 5 minutes duration respectively.

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The appearance of the spectrum in the region $\lambda 4500$—$\lambda 3900$ photographed on Fuess instrument is shown in three strips *a*, *b* and *c* in Plate IA. They correspond respectively to spectra taken with different primary voltages 60,100 and 140 of the transformer. At the lowest voltage the bands appear sharp and are clearly degraded towards red. On increasing the voltage, it was observed that many more new bands appear which are closely spaced. Under these conditions more atomic lines of iodine also appear simultaneously. Plate IB is the reproduction of the spectrum excited with 220 Volts of the primary of the transformer and was recorded on the Littrow spectrograph. Measurements of individual band heads in the region $\lambda 4420$—$\lambda 3965$ on a number of plates recorded on the above two instruments agree well with in 2 cm $^{-1}$. Out of 230 band heads measured in this region, the data of about 80 band heads coincide very well with those reported by Venkateswarulu. In Table I are reported the wavenumber data of the newly recorded band heads about 150 in number with the visual estimates of their intensities.

TABLE I

Authors wave number	Int.	Assignment v', v''	Calculated wave number	Obs.—Cal.
22623	1	1,33	22622	+1
22690	2	3,35	22696	−6
22726	1	0,30	22728	−2
22772	3	5,37	22775	−3
22798	1	4,35	22795	+3
22802	1	0,29	22802	0
22823	2	3,33	22823	0
22862	3	2,31	22859	+3
22878	2	0,28	22877	+1
22887	1	3,32	22890	−3
22895	2	5,35	22894	+1
22903	3	1,29	22903	0
22930	1	2,30	22931	−1
22960	3	3,31	22959	+1
22978	1	1,28	22979	−1
23005	3	2,29	23004	+1
23045	4	10,41	23048	−3
23050	6	11,43	23052	−2
23055	4	1,27	23056	−1
23072	4	8,37	23067	+5
23079	4	2,28	23079	0
23089	4	5,32	23089	0
23103	5	3,29	23104	−1
23115	7	0,25	23116	−1
23121	4	6,33	23120	+1
23144	4	11,41	23143	+1
23159	6	2,27	23157	+2
23178	8	3,28	23180	−2

TABLE I (contd.)

Authors wave number	Int.	Assignment v',"v	Calculated wave number	Obs.-Cal.
23222	9	9,36	23222	0
23236	8	2,26	23237	−1
23244	10	11,39	23244	0
23284	10	0,23	23284	0
23287	10	7,32	23285	−2
23307	10	5,29	23302	−5
23329	7	6,30	23327	−2
23333	9	3,26	23337	−4
23355	10	4,27	23357	−2
23379	9	8,32	23381	−2
23391	8	12,38	23392	−1
23409	6	9,33	23410	−1
23415	8	11,36	23412	+3
23422	6	7,30	23425	−3
23430	5	13,39	23431	−1
23436	5	4,26	23436	0
23444	10	11,39	23444	0
23450	8	8,31	23450	0
23481	7	9,32	23477	+4
23499	7	3,24	23502	−3
23509	5	12,36	23506	+3
23518	6	4,25	23518	0
23526	8	14,39	23524	+2
23549	8	9,31	23546	+3
23560	7	15,40	23565	−5
23575	2	2,22	23575	0
23609	3	16,41	23607	+2
23653	2	1,20	23655	−2
23664	2	2,21	23665	−1
23676	6	3,22	23675	+1
23687	5	4,23	23687	0
23705	5	19,45	23703	+2
23711	3	6,25	23715	−4
23728	5	13,34	23723	+5
23733	3	7,26	23731	+2
23748	7	1,19	23749	−1
23753	3	14,35	23753	0
23758	3	2,20	23756	+2
23773	5	4,22	23775	−2
23799	2	6,24	23798	+1
23803	2	11,36	23808	−5
23827	8	12,31	23830	−3
23848	2	15,35	23845	+3
23851	3	2,19	23850	+1

TABLE I (ontd.)

Authors wave number	Int.	Assignment v',v''	Calculated wave number	Obs.—Cal.
23874	3	5,22	23874	0
23894	3	7,24	23896	−2
23900	2	12,30	23902	−2
23910	5	8,25	23909	+1
23917	5	20,42	23918	−1
23928	6	13,31	23924	+4
23934	6	16,35	23936	−2
23942	6	1,17	23941	+1
23947	2	2,18	23945	+2
23981	2	7,23	23982	−1
23996	4	13,30	23995	+1
24003	2	9,25	24005	−2
24010	3	20,40	24014	−4
24017	3	10,26	24019	−2
24032	5	11,27	24034	−2
24045	3	3,18	24045	0
24054	2	4,19	24049	+5
24062	2	6,21	24061	+1
24079	4	8,23	24079	0
24092	4	14,30	24088	+4
24115	2	11,26	24114	+1
24126	3	12,27	24128	−2
24145	5	4,18	24145	0
24149	5	5,19	24148	+1
24166	1	8,22	24166	0
24175	4	9,23	24175	0
24206	2	12,26	24208	−2
24223	3	13,27	24222	+1
24237	6	14,28	24237	0
24244	2	1,14	24244	0
24249	2	0,13	24246	+3
24254	2	7,20	24250	+4
24280	2	11,24	24279	+1
24291	2	17,31	24291	0
24302	2	13,26	24301	+1
24345	6	2,14	24344	+1
24350	4	1,13	24346	+4
24379	2	13,25	24383	−4
24396	1	14,26	24394	+2
24407	1	15,27	24406	+1
24422	3	20,33	24422	0
24447	5	3,14	24445	+2
24459	2	12,23	24459	0
24469	3	19,31	24470	−1

TABLE I (contd.)

Authors wave number	Int.	Assignment v',v''	Calculated wave number	Obs.—Cal.
24480	1	1,12	24484	−4
24490	2	15,26	24486	+4
24534	5	7,17	24536	−2
24543	5	4,14	24544	−1
24552	4	3,13	24549	+3
24561	4	1,11	24562	−1
24583	2	2,12	24585	−2
24637	3	6,15	24638	−1
24648	3	4,13	24649	−1
24669	1	1,10	24672	−3
24681	1	0,9	24682	−1
24688	1	3,12	24685	+3
24735	2	8,16	24732	+3
24749	1	5,13	24747	+2
24798	1	0,8	24795	+3
24819	2	11,18	24822	−3
24827	2	9,16	24828	−1
24831	3	8,15	24833	−2
24846	3	6,13	24845	+1
24874	2	3,10	24873	+1
24900	1	1,8	24896	+4
24966	2	4,10	24972	−6
24997	1	2,8	24997	0
25015	1	1,7	25011	+4
25032	1	9,14	25031	+1
25043	2	8,13	25040	+3
25071	1	5,10	25071	0
25084	1	4,9	25084	0
25097	1	3,8	25097	0
25112	1	2,7	25112	0
25180	1	5,9	25182	−2
25193	1	4,8	25196	−3
25212	1	3,7	25212	0

ANALYSIS

Waser and Wieland (1947) were the first to propose the following vibrational quantum formula for the bands of iodine molecule in the blue violet region.

$$\nu = 25757.2 + (101.88v' - 0.34v'^2) - (126.59v'' - 0.755v''^2 - 0.0033v''^3).$$

However, they have not published their experimental data or the vibrational analysis of the bands. Venkateswarulu (1951) reported the classification of about

80 bands of this system on the basis of the above formula. In his analysis the scheme consists of assignments of bands with $v' = 0$ to 11 and $v'' = 9$ to 38. The wavenumbers of these bands are in close agreement with those obtained by the authors. Further, the agreement between the observed and calculated wavenumbers for all the 80 bands is remarkably good. Hence, it is concluded that the vibrational formula proposed by Waser and Wieland represents very well all the 80 bands assigned by Venkateswarulu. However, it is observed that there are a large number of gaps in the vibrational array proposed by him. It is possible to assume that the new bands, 150 in number, obtained in the present investigations could very well form part of this system. On this basis, the above vibrational scheme was extended to include the new bands. It was found possible that all the bands in the region $\lambda 4420$—$\lambda 3965$ could be analysed as belonging to a single system whose vibrational formula is the same as that proposed by Waser and Wieland. The vibrational assignments of these new heads were shown in column 4 of Table I. The observed wavenumbers of all these newly assigned band heads were compared with those calculated on the basis of the above formula and their differences were indicated in the last column. The extended vibrational analysis consists of assignments of bands with $v' = 0$ to 20 and $v'' = 7$ to 45.

The intensity distribution of bands of this system is indicated in Table II. It can be seen that most of the strongest bands of the system belong to $v' = 0$ to 6 progressions and the progressions with $v'=0$ to 5 are more fully developed. The intensity distribution in the system closely corresponds to a typical Condon parabola which is to be expected for values of $\omega_e' = 102.2\text{cm}^{-1}$ and $\omega_e'' = 126.6$ cm^{-1}.

ELECTRONIC STATES

The vibrational constants of the lower state of this system suggest that this is to be identified with the upper state $^3\Pi_{0u}{}^-$ of the visible absorption bands. The upper state of the system was already attributed to the molecular electronic configuration $\sigma_g{}^2\pi_x{}^2\pi_y{}^4\sigma_u{}^2 - {}^3\Sigma^-_g$, $^1\Sigma^-_g$, $^1\Delta_g$ of which $^3\Sigma^-_g$ is expected to be lower in energy. These states give rise to $(0_g^-, 1_g)$, 0_g^- and 2_g respectively in Hund's case C coupling. This system designated as $D-B$ was tentatively ascribed to the transition $^1\Sigma_g^-(0_g^-)$ to $^3\Pi_{0u}(0_u^-)$ by Haranath and Rao. Recently Mathieson and Rees have discussed the dissociation products of a group of electronic levels of iodine molecule lying at 40,000 to 55,000 cm^{-1} by consideration of the ionic attractive forces operating. They found that the neighbouring states E and D (D and C according to Haranath and Rao) at $\nu 41411$ and $\nu 39293$ respectively dissociate into the same products of ions $^3P_2(\text{I}^-)$ and $^1S_0(\text{I}^-)$. They assigned the state at $\nu 41411$ the upper electronic level of the blue violet emission band system of iodine to the term $^3\Sigma_g^-(0_g^-)$ arising out of the configuration (2242). Hence it seems reasonable to assign the $D-B$ system to the electronic transition $^3\Sigma_g^-(0_g^+)-$

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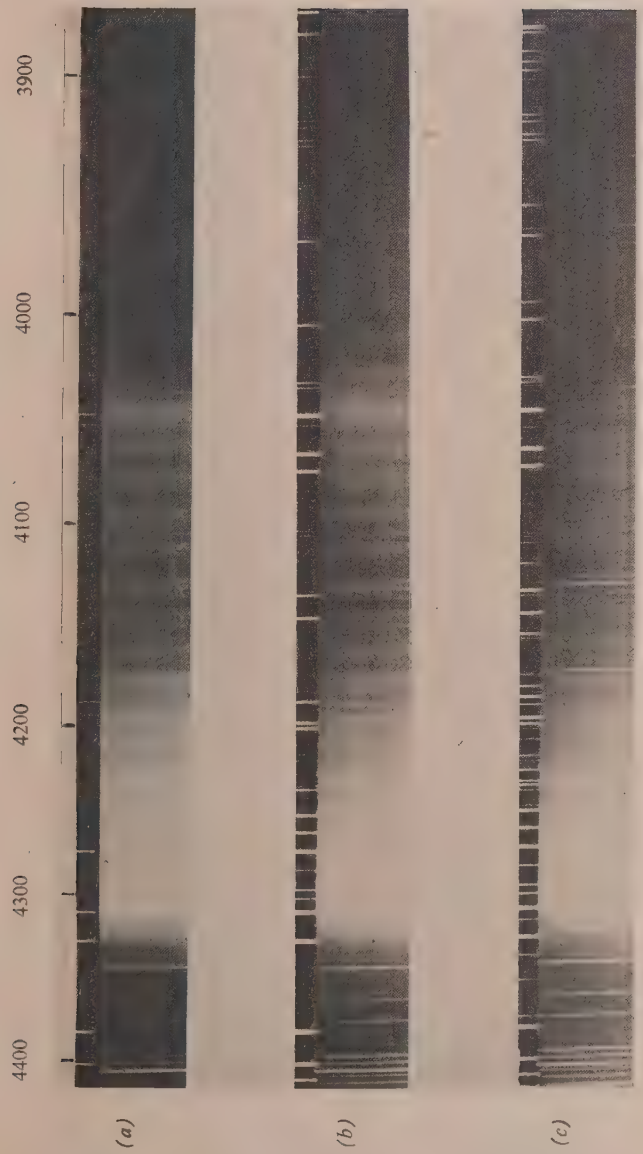

Emission spectra of iodine excited in condensed discharge from a transformer at different primary voltages. Fuess spectrograms. *(a)* 60 volts, *(b)* 100 volts, *(c)* 140 volts.

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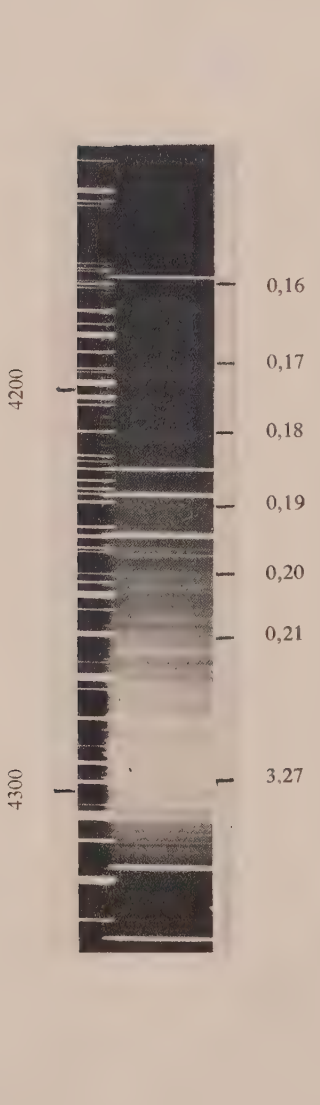

Emission spectrum of iodine excited in condensed discharge from a transformer at 220 volts primary. Glass Littrow spectrograms.

Intensity distribution of the emission band system of iodine.

v' \ v''	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
0		1	1	3	2		2	4	4	5	7	7	7	8	8	8	10	9	7	3	3	2	1	1															
1	1	1	2	1	4	1	4	2	4	4	5	7	7	7	7	7	9	10	7	4	4	1	1				1											
2	1	1			1	2	1	6	6			2	3	3	2	2	8	7	7	8	6	4	3	1	2													
3	1	1	2	2		1	4	5	6			3		3	5	6		7	7	9	10	8	5		3	2	2	1	1	1								
4		1	1	2			3	5	5			5	2	4	6	5	5		6	5	7	10							1	1								
5			1	1			1	3		5			5			3	6		3	8			10	9		5			2		2							
6							2	3	3	5					2	3	3	2	3					7	10	8	4												
7							3	3			5			2		2	2	3	2	5				6		10		6											
8							2	2	3	3	3					1	4	4	5				2		8	9		9			4	3							
9								1		2					4		4	4	2	5					8	7	8	9		9		6							
10										2		2					2			3							5	9						5	4				
11												2						2	5	2	5			2					6			10			4		6		
12																	2			2	3			2	8				5		8							
13																			2	2	3			4	6			5					5					
14																				1		6		4	3				3				8					
15																				2	1	4			4			5	2					7				
16																										3			6						3				
17																									2													
18																																							
19																									3											6		5	
20																												3						3		6			

$^3\Pi_{0^-}$ (0^-) in which case the selection rules of Hund's cases *C* and *B* coupilngs hold good simultaneously.

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15

ON ZERO MASS MESON-MESON SCATTERING

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ABSTRACT. The forward scattering matrix elements for the scattering of two mesons (zero mass) has been calculated from pair reproduction cross section by the method of analytic continuation. This has been compared with the Feynaman matrix elements to the required order. By comparing the results of the two methods, the value of the counter $\lambda\phi^4$ term has been evaluated.

INTRODUCTION

Besides primitive divergencies, there is a class of divergences (comparable to photon-photon scattering divergency) peculiar to meson-nucleon interactions. The degree of divergence D for the process is determined by the well known relation

$$D = 4 - 3/2\ F_e - B_e$$

where F_e = number of external fermion lines

Be = number of external Boson lines.

Thus closed loops of fermions with three and four vertices of bosons are divergent. For photons and pseudoscalar mesons which are of importance in physics, a closed loop with three vertices have zero matrix element. But the four-vertex diagram is permissible and also possible giving rise to processes like photon-photon or meson-meson scattering. Therefore, suitable counter term (i) $\lambda A_\mu{}^4$ or (ii) $\lambda\phi^4$, where A_μ is the photon and ϕ the meson field operator, are to be added to the interaction Hamiltonian. For electrodynamics, gauge invariance forbids the occurence of the term $\lambda A_\mu{}^4$ in the Lagrangian; as a consequence, terms proportional to it can be dropped since they are non-gauge-invariant. Fortunately, however, if one calculates the matrix elements there is no divergence if the contribution for all the three basic diagrams are added up, as shown by Jauch and Robrlich (1955).

But for meson-meson scattering, gauge invariance is not available. This is the first (and only) divergent process which is not eliminated by a renormalisation of mass or coupling constant in pseudoscalar theory. Therefore a counter term $\lambda\phi^4$ is essential. However the exact value of λ even in the lowest order has not been calculated since no method exists as to its unambiguous evaluation, as has been pointed out by Schweber, Bethe and de' Hoffmann (1955). Therefore, it is interesting to be able to complete this counter term, to see to what extent the absence of gauge invariance can be compensated by alternate mode of thought.

FORMULATION OF THE PROBLEM

We shall use natural units $\hbar = c = 1$.

Let a pseudoscalar boson field ϕ and a fermi field ψ interact, the Hamiltonian in interaction representation being given by,

$$Hint = ig \int d^3x \, \bar{\psi}\gamma_5\psi\phi$$

The fourth-order term of S-matrix which describes the effects under consideration is given by the Feynman diagram, (Fig. 1)

or by the integral

$$S^{(4)} = -\frac{1}{64} g^4 \int\int\int\int d^4x_1 d^4x_2 d^4x_3 d^4x_4 \phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)$$

$$T_r\{\gamma_5 \; S_F(x_2 - x_1)\gamma_5 S_F(x_3 - x_2)\gamma_5 \; S_F(x_4 - x_3)\gamma_5 \; S_F(x_1 - x_4)\} \qquad \ldots \quad (1)$$

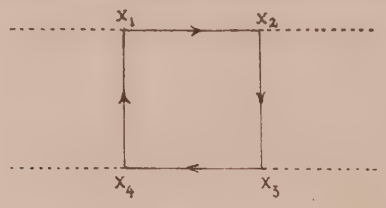

Fig- 1

$S_F(x)$ being the propagation function of the fermi field (mass $= m$)

$$S_F(x) = -\frac{2i}{(2\pi)^4} \underset{\epsilon \to 0^+}{\text{Lt}} + \int d^4p \ldots \frac{i\gamma \cdot p - m}{p^2 + m^2 - i\epsilon} e^{-ip.x}$$

$$p \cdot x = \vec{p} \cdot \vec{r} - p_0 x_0.$$

The transition to momentum space with

$$\phi(x) = \int \phi(k) e^{ik.x} d^4k \qquad \ldots \quad (1a)$$

yields,

$$S^{(4)} = -\frac{i}{4}\left(\frac{g^2}{4\pi}\right)^2 \int d^4x \int d^4k_1 \int d^4k_2 \int d^4k_3 \int d^4k_4 \, \phi(k_1)\phi(k_2)\phi(k_3)\phi(k_4).$$

$$. e^{i(k_1+k_2+k_3+k_4) \cdot x} \frac{1}{3} G(k_1 k_2 k_3 k_4) \qquad \ldots \quad (2)$$

where

$$G(1234) = T^{(1)}(1234) + T^{(2)}(1, 2, 4, 3) + T^{(3)}(1, 3, 24) \qquad \ldots \quad (2a)$$

and

$$T^{(1)}(1234) = \frac{1}{i\pi^2}\int d^4p \,.\, Tr.\{\gamma_5 S_F(p)\gamma_5 S_F(p-k_2)\gamma_5 S_F(p-k_2-k_3)\gamma_5 S_F (p-k_2-k_3-k_4)\}$$

$$T^{(2)} = T^{(1)}(k_2 \Longleftrightarrow k_4)$$

$$T^{(3)} = T^{(1)}(k_2 \Longleftrightarrow k_3) \qquad \ldots \quad (3)$$

It is easily seen that the divergent term is entirely contained in the terms proportional to $(p^2)^2$ in the numerator and is logarithmically divergent. Therefore subtraction any term whatsoever, containing the log-divergent term shall eliminate this divergence.

To get round this difficulty we first note that the quantity we wish to subtract is essentially a constant independent of the scattering angle. So our problem will be considerably simplified if we can compute the matrix elements for forward scattering only. We let,

$$k_1 = k; \quad k_3 = -q; \quad k_2 = -k; \quad k_4 = q$$

Then only invariant that can be constructed is $k.q$, and in a c.m. system, $k\,.q = -2\omega^2$ for forward scattering. So we write,

$$G(k, q) = G(k\,.q) = G(\omega^2, 0) = G(t, 0) \qquad \ldots \quad (4)$$

where $t = w^2/m^2$ for convenience.

The matrix element is a function of the invariant 't' $= -2k\,.\,q/4m^2$. We can further separate the real and imaginary part of the Function

$$G(t, 0) = a_1(t) + ia_2(t) \qquad \ldots \quad (5)$$

The imaginary part $a_2(t)$ is related to the pair production cross-section.

The unitarity of S-matrix, makes it possible to write the total transition probability for the production of a pair of fermions by two messons.

$$P = -2R_e[\psi_i,\ S^{(4)}\psi_i]$$

$$= -\left[\frac{2}{V^2}\int d^4x\right]\left(\frac{g^2}{4\pi}\right)^2 \frac{1}{t}\ \text{Im.}\, G(t, 0) \qquad \ldots \quad (6)$$

This is evaluated by the usual substitution, (See reference R. Karplus and M. Neuman (1951)).

$$\phi(\vec{k}, k_0) \rightarrow V(2\,|\,k\,|\,V)^{-\frac{1}{2}}[a(\vec{k})\delta(k_0 - |\,\vec{k}\,|) - a^{\dagger}(-\vec{k})\delta(k_0 + |\,\vec{k}\,|)$$

$$\int \vec{dk} \rightarrow \frac{1}{V}\sum_{k}$$

where $a(\vec{k})$ and $a^{\dagger}(\vec{k})$ are the anihilation and creation operators and V a large but finite volume. The total cross-section of pair production by two mesons of momentum

$$\vec{k}_1 = \vec{k}\,; \quad \vec{k}_2 = -\vec{k}, \quad |\vec{k}_1| = |\vec{k}_2| = \omega \qquad \text{is then}$$

$$\sigma_{pair}(t) = -2(g^2/4\pi)^2 \frac{1}{m^2 t} \text{ Im } G(t, 0)$$

Thus

$$a_2(t) = \frac{1}{(g^2/4\pi)^2} \frac{m^2 t}{2} \sigma_{pair}(t) \qquad \ldots (7)$$

Following the same procedure, the probability for meson-meson scattering is

$$P = \frac{2}{V^2} \int d^4x \left(\frac{g^2}{4\pi}\right)^4 \frac{1}{128\pi^2} \frac{1}{m^2 t} \int d\Omega(\vec{k}) \, |G(t)|^2 \qquad \ldots (8)$$

when the diff. scattering cross-section in the forward direction in c.m. system is

$$\frac{d\sigma}{d\Omega}(t, 0) = \left(\frac{g^2}{4\pi}\right)^4 \frac{1}{64\pi^2 m^2 t} \, |G(t, 0)|^2$$

$$= \left(\frac{g^2}{4\pi}\right)^4 \frac{1}{64\pi^2 m^2 t} \, |a_1 + i a_2|^2. \qquad \ldots (9)$$

We see that pair production cross-section $\sigma_{pair}(t)$ shall enable us to write $a_2(0, t)$. We shall then resort to the method of analytic continuation, suggested by Toll (1952) and calculate $a_2(t, 0)$.

PAIR PRODUCTION CROSS-SECTION

The matrix element for pair production is

$$\langle p\, p' \mid M \mid k_1 k_2 \rangle = -\frac{ig^2}{(2\pi)^2} \frac{m}{\sqrt{\omega_p \omega_{p'} 2\omega_1 2\omega_2}} \cdot$$

$$\bar{u}(p)\left[\gamma_5 \frac{ir \cdot \overline{p-k_1} - m}{2p \cdot k_1} \gamma_5 + \gamma_5 \frac{ir \cdot \overline{p-k_2} - m}{2p \cdot k_2} \gamma_5\right] v(p') \qquad \ldots (10)$$

arising from the crossed and uncrossed Feynman diagrams. The total scattering cross-section can be evaluated in standard way and one gets.

$$\sigma_{pair}(t) = 8\pi \left(\frac{g^2}{4\pi}\right)^2 \frac{1}{m^2 t} \left[\log \frac{1+\left(1-\frac{1}{t}\right)^{\frac{1}{2}}}{1-\left(1-\frac{1}{t}\right)^{\frac{1}{2}}} - 2\left(1-\frac{1}{t}\right)^{\frac{1}{2}} \right], \quad t > 1$$

$$= 0 \qquad (t < 1) \qquad \ldots \quad (11)$$

Equation (7) now gives

$$a_2(t) = -4\pi \left[\log \frac{1+\left(1-\frac{1}{t}\right)^{1/2}}{1-\left(1-\frac{1}{t}\right)^{1/2}} - 2\left(1-\frac{1}{t}\right)^{1/2} \right] ; \; t > 1$$

$$= 0 \; ; \; t < 1 \qquad \ldots \quad (12)$$

However, these expressions hold good only for positive and real t.

For the use of analytic continuation we must know the value of Im. $G(t, 0)$ for $t < 0$. To find this out we resort to the Feynman diagrams as depicted in Figs. 2(a), 2(b), and 2(c) which gives respectively $T^{(1)}$, $T^{(2)}$ and $T^{(3)}$ of equation 2(*a*) with $k_1 = -k_2 = -k$; $k_3 = -k_4 = -q$

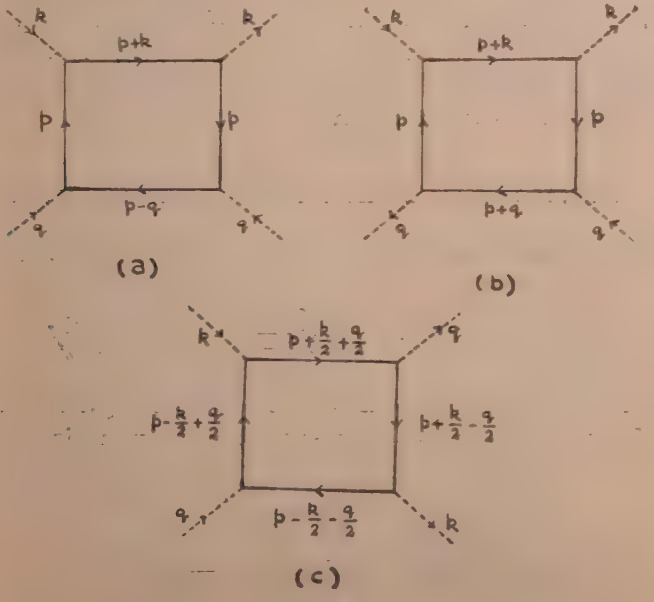

Fig. 2

From general four-momentum conservation we label the integral fermion lines as shown. Figure 2(c) we have shifted the value of 'p' which does not bring in any surface term, since the matrix element is only log. divergent. Inspection of Figs. 2(a) and 2(b) shows that

$$T^{(1)} = T^{(1)}(k.q) \quad \ldots \quad (13a)$$

$$T^{(2)} = T^{(1)}(k,-q) = T^{(1)}(-k.q) \quad \ldots \quad (13b)$$

$$\therefore \quad T^{(1)} + T^{(2)} = T^{(1)}(k.q) + T^{(1)}(-k.q) \quad \ldots \quad (13c)$$

This means that the matrix elements of $T^{(2)}(k, q)$ can be obtained from $T^{(1)}(k, q)$ by replacing q by $-q$. Since the contribution from each diagram must be a function of the only available invariant $k.q$, equations 13(b) and 13(c) follows.

In diagram, Fig. 2(c), we note immediately that,

$$T^{(3)}(k, q) = T^{(3)}(k, -q) = T^{(3)}(-k, q) \quad \ldots \quad (14)$$

Thus

$$G(t, 0) = G(-t, 0) \quad \ldots \quad (15)$$

These symmetry properties are adequate to calculate the Matrix elements for forward scattering from pair production cross-section by analytic continuation. The S-matrix matrix elements can also be computed directly by Feynman method. The results from these two methods shall be compared. Retaining only those terms that can be obtained from analytic continuation, the counter renormalisation term for a finite S-matrix can be found out. We shall first make the necessary analytic continuation, in the next section and in the succeeding section, find the S-matrix elements.

METHOD OF ANALYTIC CONTINUATION

Following Rohrlich and Gluckstern (1952), we consider Cauchy's Theorem,

$$f(x) = \frac{1}{2\pi i} \oint \frac{f(z')}{z'-z}\, dz' \quad \ldots \quad (16)$$

Let z be on the real axis, $z = t$ and assume that $f(z)$ is regular for $\mathrm{Im}.(z) \geq -\epsilon$; $\epsilon > 0$. We can choose the path of integration as shown in Fig. 3 and write

$$f(t) = \frac{1}{2\pi i} P \int_{R}^{+R} \frac{f(t')}{t'-t}\, dt' + \frac{1}{2} f(t) + \frac{1}{2\pi i} \int_{R} \frac{f(z')}{z'}\, dz' \quad \ldots \quad (17)$$

where in the last integral t has been neglected in the denominator, since for the contour $R; |z'| \gg t$ everywhere. We further assume that $f(z')/z'$ is regular at $z' = 0$, so that

$$\int_R \frac{f(z')}{z'}\, dz' = -\int_{-R}^{+R} \frac{f(t')}{t'}\, dt' \qquad \ldots \quad (18)$$

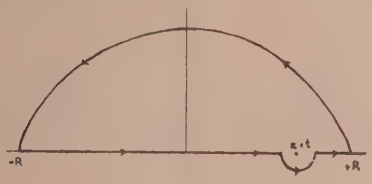

Fig. 3

Separating $f(t)$ into its real and imaginary parts, we obtain with $R \to \infty$

$$\text{Re}\, f(t) = \frac{t}{\pi} P \int_{-\infty}^{+\infty} \frac{Im.f(t')}{t'(t'-t)}\, dt' \qquad \ldots \quad (19)$$

We identify $f(t)$ with $G(0, t)$ and since,

$$G(0, t) = G(0 - t)$$

we get

$$Re\, G(0, t) = 2t^2 \frac{P}{\pi} \int_0^{\infty} \frac{\text{Im}\,.\, G(0, t)}{t'^2 - t^2} \frac{dt'}{t'.} \qquad \ldots \quad (20)$$

Thus we get

$$a_1(t) = -\,8t^2 P \int_1^{\infty} \left[\log \frac{1 + \left(1 - \frac{1}{t'}\right)^{\frac{1}{2}}}{1 - \left(1 - \frac{1}{t'}\right)^{\frac{1}{2}}} - 2\left(1 - \frac{1}{t'}\right)^{\frac{1}{2}} \right] \frac{dt'}{t'} \cdot \frac{1}{t'^2 - t^2}$$

$$= 8t^2 P \int_0^1 \frac{p'dp'}{1 - t^2 p'^2} \left[\log \frac{1 - (1-p')^{\frac{1}{2}}}{1 + (1-p')^{\frac{1}{2}}} + 2(1 - p')^{\frac{1}{2}} \right] \qquad \ldots \quad (21)$$

where we have put $t' = \dfrac{1}{p'}$

These integrals can be evaluated in straight forward way. But for sake of comparison, we shall make the following substitutions.

Integrating by parts,

$$a_1(t) = 4P \int_0^1 \left(\frac{1}{(1-p')^{\frac{1}{2}} p'} - \frac{1}{(1-p')^{\frac{1}{2}}} \right) \log (1-t^2 p'^2) dp'$$

Letting

$$\sqrt{1-p'} = u, \quad -\frac{1}{2} \frac{dp'}{\sqrt{1-p'}} = du$$

$$a_1(t) = 8P \int_{0=2}^{1} \left(\frac{1}{1-u^2} - 1 \right) \log \left[1 - 16t^2 \left(\frac{1-u^2}{4} \right)^2 \right] du$$

$$= 4P \int_{-1}^{+} \left(\frac{1}{1-u^2} - 1 \right) \log \left[1 - 16t^2 \left(\frac{1-u^2}{4} \right)^2 \right] du$$

$$= 8P \int_0^1 \left(\frac{1}{4x} - 1 \right) [\log (1 - 4tx(1-x)) + \log (1 + 4tx(1-x))]$$

with $\quad x = \frac{1+u}{2}, \qquad \ldots (22)$

Evaluating

$$\frac{1}{8} a_1(0, \omega) = \left(\sinh^{-1} \frac{\omega}{m} \right)^2 - 2 \left(1 + \frac{m}{\omega} \right)^{\frac{1}{2}} \sinh^{-1} \frac{\omega}{m}$$

$$= \begin{cases} \left(\sin^{-1} \frac{\omega}{m} \right)^2 - 2 \left(\frac{m^2}{\omega^2} - 1 \right)^{\frac{1}{2}} \sin^{-1} \frac{\omega}{m}; & 0 < \omega < m \\ \left(\cosh^{-1} \frac{\omega}{m} \right)^2 - \frac{\pi^2}{4} - 2 \left(1 - \frac{m^2}{\omega^2} \right)^{\frac{1}{2}} \cosh^{-1} \frac{\omega}{m}; & \omega > m. \end{cases} \quad \ldots (23)$$

$$\frac{1}{8} a_2(0, \omega) = -\pi \left\{ \cosh^{-1} \frac{\omega}{m} - \left(1 - \frac{m^2}{\omega^2} \right)^{\frac{1}{2}} \right\}; \quad \omega > m$$

$$= 0; \quad \omega < m. \qquad \ldots (24)$$

Using equation (9), one can now calculate meson-meson scattering cross-section in the forward direction. This is what a physicist would have done, had Feynman method not been known, analytic contuation methods were known.

DIRECT EVALUATION OF MATRIX ELEMENTS

One now proceeds to calculate directly Matrix elements $G(kq)$ of equation (2), using the Feynman's diagrams Figs. 2(a), (b) and (c). Even in case of forward scattering, the calculations are extremely lengthy and tedious. The proceedure and details of calculation have been outlined by Jost Luttinger and Slotnick (1950). We merely quote the results. (the details of calculations can be supplied on request).

$$G(k_1q) = 12D_\infty - 8\int_0^1 \left(\frac{1}{4y} - 1\right) \log\left(1 - \frac{2kq}{m^2}\, y(1-y)\right)$$

$$+ 8\int_0^1 \left(\frac{1}{4y} - 1\right) \log\left(1 + \frac{2kq}{m^2}\, y(1-y)\right)$$

where $$D_\infty = \frac{1}{i\pi^2}\int d^4p \cdot \frac{(p^2)^2 + 2m^2p^2 + m^4}{(p^2 - m^2)^4} \qquad \ldots \quad (25)$$

Letting $2k.q = -4\omega^2 = -4m^2t$, we see that $G(k.q) - 12D_\infty = G_f$ gives correctly the values of a_1 and a_2 deduced before. Referring to equation (2) we see that, in general,

$$S^{(4)} = -\frac{i}{12}\left(\frac{g^2}{4\pi}\right)^2 \int d^4x \int d^4k_1 \ldots d^4k_4\; e^{i(k_1+k_2-k_3-k_4)\cdot x}\; \phi(k_1)\phi(k_2)\phi(k_3)\phi(k_4).$$

$$[12D_\infty + G_f(k_1k_2k_3k_4)]. \qquad \ldots \quad (26)$$

The first term (which is diverent) is $-i\left(\frac{g^2}{6\pi}\right)^2 D_\infty \int d^4x\phi^4(x)$. since the momentum space transform is given by (1a).

Thus if we start with the interaction Hamiltonian density

$$H_{int} = ig\bar{\psi}\gamma\gamma_5\psi\phi - \left(\frac{g^2}{4\pi}\right)^2 D_\infty\phi^4(x) \qquad \ldots \quad (27)$$

then, the contribution due to the second term in the first order is

$$\frac{(-i)^1}{11}\left(\frac{g^2}{4\pi}\right)^2 D_\infty \int \phi^4(x)d^4x = +i\left(\frac{g^2}{4\pi}\right) D_\infty \int d^4x\phi^4(x)$$

which cancels the first term in (26). So the finite $S^{(4)}$ is now given by

$$S^{(4)} = -\frac{i}{12}\left(\frac{g^2}{4\pi}\right)^2 \int d^4x \int \quad \ldots \quad G_f(k_1k_2k_3k_4)$$

This G_f in the forward direction shall now give

$$G_f(0, t) = a_1 + ia_2$$

which can be derived by analytic continuation method.

Thus the contact renormalisation term $\lambda\phi^4$ that must be subtracted from the interaction Hamiltonian density is unambiguously determined with

$$\lambda = \left(\frac{g^2}{4\pi}\right)^2 \frac{1}{i\pi^2} \int \frac{d^4p}{(p^2+m^2-i\epsilon)^4} \quad ((p^2)^2+2m^2p^2+m^4)$$

$$= \left(\frac{g^2}{4\pi}\right)^2 \left[\underset{\Delta\to\infty}{\alpha t} \log \frac{\Delta^2+m^2}{m^2} - 1 \right] \qquad \ldots \quad (29)$$

The low energy theorem then turns out to be

$$\underset{t\to 0}{\alpha t} \quad G(0, t) = 0$$

We have used the method of analytic continuation which can also be derived from dispersion relations. Thus it seems that the causality requirements may as well provide the clue for a low energy theorem for meson-meson scattering. An application of the general dispersion relation to evaluate the low energy limit for π–π scattering is in progress.

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16

FORCE CONSTANTS FOR UNLIKE MOLECULAR INTERACTIONS ON EXP-SIX MODEL FROM INTER-DIFFUSION

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ABSTRACT. Force constants for unlike molecular interactions for the systems Ne–A, Ne–Kr, A–Kr, He–A, A–Xe, He–Xe, He–Kr and Ne–Xe have been determined on the exponential six model from temperature dependence of inter-diffusion coefficients. To simplify matters, the values of α_{12} were taken to be those obtained from the temperature dependence of thermal diffusion or from the combination rules and the method of intersection was employed to give ϵ_{12} and $(r_m)_{12}$. The force constants, thus obtained, have been compared with the values obtained from other methods and satisfactory agreement has been obtained. These force constants have been used to calculate the thermal diffusion factors at different temperatures and reasonable agreement has been obtained except in the case of A–Kr.

INTRODUCTION

The inter-molecular potentials for like molecules have been determined accurately for many molecules by a large number of workers. For this purpose, various transport properties of gases, specially viscosity, have been utilised. However, there is considerable uncertainty in the values of unlike force constants for most of the molecular pairs, as there is lack of suitable accurate experimental data over a large temperature range. The transport properties of gas mixtures depend on both like and unlike force parameters, and in cases of viscosity and thermal conductivity the like molecular interaction tends to mask the effect of unlike interactions. In case of thermal diffusion, the masking is reduced, and for inter-diffusion it is insignificant. Unfortunately, until quite recently, sufficiently accurate inter-diffusion data were not available over an extended temperature range. On the other hand, thermal diffusion data being readily available, have been utilised by Srivastava and Madan (1953), Saxena (1955), Srivastava and Srivastava (1957), and Srivastava (1957), for the calculation of the unlike force parameters. Srivastava and Srivastava (1959), and Barua (1959) combined inter-diffusion data with viscosity data to evaluate unlike force constants, which enables even one or two values of the diffusion constant to be utilised.

Recently, several workers (Strehlow, 1953; Bunde 1955; Rumpel, 1955; Srivastava and Srivastava, 1959; Srivastava, 1959; Srivastava and Barua 1959)

have determined D_{12} over a wide range of temperatures and utilised it to determine the unlike force constants on Lennard-Jones 12 : 6 model. In the present paper the values of inter-diffusion coefficients by Srivastava and Srivastava (1959), Srivastava (1959), and Srivastava and Barua (1959) have been used to determine unlike force parameters on the exp-six model. This is of considerable importance as the combination rules so far given are largely emperical and cannot therefore be considered satisfactory.

DETERMINATION OF THE FORCE PARAMETERS

On the Exp-Six model, the potential $\phi(r)$ between two molecules, when separated by a distance r, is given by

$$\phi(r) = \frac{\epsilon}{1 - \frac{6}{\alpha}} \left[\frac{6}{\alpha} \, e^{\alpha \left(1 - \frac{r}{r_m}\right)} - \left(\frac{r_m}{r}\right)^6 \right] \qquad \ldots (1)$$

where ϵ is the depth of the potential energy minimum, r_m is the separation distance for the energy minimum and α is the parameter which gives the steepness of the repulsion energy. The molecular parameters are denoted by ϵ_{ij} $(r_m)_{ij}$ and α_{ij}, where i, j denote the two interacting molecules.

Two sets of combination rules have been recently proposed which enable us to calculate the unlike force parameters in terms of like parameters. The combition rules given by Mason and Rice (1954) are

$$\left[\frac{\epsilon_{12}}{1 - \frac{6}{\alpha_{12}}} \, \frac{6}{\alpha_{12}} \, e^{\alpha_{12}} \right] = \left[\left\{ \frac{\epsilon_{11}}{1 - \frac{6}{\alpha_{11}}} \cdot \frac{6}{\alpha_{11}} \, \epsilon^{\alpha_{11}} \right\} \left\{ \frac{\epsilon_{22}}{1 - \frac{6}{\alpha_{22}}} \cdot \frac{6}{\alpha_{22}} \, e^{\alpha_{22}} \right\} \right]^{\frac{1}{2}}$$

$$\frac{\alpha_{12}}{(r_m)_{12}} = \frac{1}{2} \left[\frac{\alpha_{11}}{(r_m)_{11}} + \frac{\alpha_{22}}{(r_m)_{22}} \right] \qquad \ldots (2)$$

$$\frac{\epsilon_{12}(r_m)^6_{12}}{1 - \frac{6}{\alpha_{12}}} = \left[\frac{\epsilon_{11}(r_m)^6_{11}}{1 - \frac{6}{\alpha_{11}}} \cdot \frac{\epsilon_{22}(r_m)^6_{22}}{1 - \frac{6}{\alpha_{22}}} \right]^{\frac{1}{2}}$$

while the following are given by Srivastava and Srivastava (1957)

$$\frac{\alpha_{12}}{(r_m)_{12}} = \frac{1}{2} \left[\frac{\alpha_{11}}{(r_m)_{11}} + \frac{\alpha_{22}}{(r_m)_{22}} \right]$$

$$\epsilon_{12} = (\epsilon_{11} \cdot \epsilon_{22})^{\frac{1}{2}}, \qquad \ldots (3)$$

$$\frac{\epsilon_{12}(r_m)^6_{12}}{1 - \frac{6}{\alpha_{12}}} = \left[\frac{\epsilon_{11}(r_m)^6_{11}}{1 - \frac{6}{\alpha_{11}}} \cdot \frac{\epsilon_{22}(r_m)^6_{12}}{1 - \frac{6}{\alpha_{22}}} \right]^{\frac{1}{2}}$$

These have been used to yield value of α_{12} where this value was not known from the thermal diffusion data.

The procedure adopted for calculating the force constants is as follows :—

The experimental value of D_{12} at different temperatures were plotted and four smoothed out values of D_{12} were taken. Theoretically, D_{12} is given by

$$D_{12} = .002628 \frac{T^{3/2}}{p(r_m)^2_{12}\,\Omega_{12}{}^{(11)*}(T_{12}{}^*)} \left[\frac{M_1 + M_2}{2M_1M_2}\right]^{\frac{1}{2}} \quad \ldots \quad (4)$$

where p is the pressure in atmospheres. $T_{12}{}^* = \frac{kT}{\epsilon_{12}}$. k being the Boltzmann's constant; and $\Omega_{12}{}^{(11)}$ is a reduced collision integral tabulated by Mason (1954), other symbols having their usual meanings. The values of α_{12} were taken from the previous determinations from thermal diffusion data, where available. In other cases it was calculated from the combination rules given by Srivastava and Srivastava (1957).

From equation (4), substituting a set of values for ϵ_{12}, the corresponding values of $(r_m)_{12}$ were found out using the value of D_{12} at a certain temperature. This was repeated with values of D_{12} at other temperatures, and in this way the values of $(r_m)_{12}$ against ϵ_{12} were plotted and curves were drawn corresponding to each temperature. Since the values of ϵ_{12} and $(r_m)_{12}$ should not vary with temperature, these curves should intersect at a single point. However, due to experimental error, several intersection points occur, fairly close to each other. The mean of all these values gives the required set of force parameters.

In the case where viscosity data on mixture were available, the values of force constants were also determined by combining the viscosity data with inter-diffusion data. The method used for this purpose is essentially the same as that used by Srivastava and Srivastava (1959). Viscosity data were taken from Rietveld, Itterbeek and vanDen Berg (1953) and Trautz and Binkele (1930).

RESULTS

For easy reference the smoothed out values of the inter-diffusion coefficient are recorded in Table I.

In Table II, are tabulated the values of the force constants obtained by the method indicated above, together with the values obtained from a combination of viscosity and mutual diffusion, and from the temperature variation of thermal

diffusion. The respective values from the different combination rules are also given for the sake of comparison.

TABLE I

Experimental values of the coefficients of inter-diffusion

Gas pairs	273°K	288°K	303°K	318°K
A–He	0.640	0.701	0.760	0.825
A–Xe	0.0943	0.102	0.114	0.128
He–Xe	0.501	0.550	0.604	0.655
Ne–A	0.276	0.300	0.327	0.357
Ne–Kr	0.223	0.240	0.266	0.284
A–Kr	0.119	0.128	0.140	0.153
He–Kr	0.556	0.605	0.659	0.720
Ne–Xe	0.186	0.202	0.221	0.244

TABLE II

Force Parameters

Gas pair		From intersection	From viscosity and diffusion	From thermal diffusion	Combination rule : Srivastava & Srivastava (1957)	Combination rules : Mason and Rice (1954)
Ne–A	α_{12}	14.18	14.18	14.18	14.35	14.17
	ε_{12}/k	64.5	66.6	67.6	68.42	73.7
	$(r_m)_{12}$	3.511	3.497	3.504	3.491	3.443
Ne–Kr	α_{12}	13.84		13.84	14.15	13.55
	ε_{12}/k	68.75		73.4	71.74	89.54
	$(r_m)_{12}$	3.725		3.720	3.710	3.549
A–Kr	α_{12}	13.61			13.61	13.52
	ε_{12}/k	128.25			129.2	132.8
	$(r_m)_{12}$	4.123			4.101	4.072
He–A	α_{12}	13.5	13.5	13.5	13.20	13.21
	ε_{12}/k	29.3	31.5	33.4	33.59	33.40
	$(r_m)_{12}$	3.523	3.504	3.471	3.484	3.488
A–Xe	α_{12}	13.4		13.4	13.58	13.44
	ε_{12}/k	173.25		170.5	168.8	178.5
	$(r_m)_{12}$	4.200		4.158	4.153	4.108
He–Xe	α_{12}	12.86	12.86		12.86	12.56
	ε_{12}/k	44.2	39.8		46.03	57.88
	$(r_m)_{12}$	3.756	3.803		3.743	3.653
He–Kr	α_{12}	12.89			12.89	12.64
	ε_{12}/k	35.0			35.23	38.73
	$(r_m)_{12}$	3.690			3.696	3.625
Ne–Xe	α_{12}	14.0		14.0	14.15	13.45
	ε_{12}/k	88.88		80.0	93.74	121.8
	$(r_m)_{12}$	3.837		3.799	3.758	3.574

COMPARISON WITH EXPERIMENT

The force constants obtained by the method of intersection are utilised to calculate the thermal diffusion factor at different temperatures. Table III gives the values of α_T, thus obtained, together with the experimental values as determined by Grew (1947) and Grew, Johnson and Neal (1954).

TABLE III

Comparison with experimental values of α_T

Gas Pairs	185°K		293°K		465°K	
	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.
Ne–A	.142	.148	.176	.174	.194	.191(a)
Ne–Kr	.220	.210	.284	.290	.319	.320(b)
A–Kr	.040	.032 .038	.108	.060 .075	.121	.080(a) .149(b)
He–A	.368	.360	.381	.380	....	....(b)
A–Xe	.016	.063	.100	.087	.179	.176(b)
He–Xe	....	....	.426	.434	.441	.434(b)
He–Kr	.397	.430	.428	.448	.440	.448(b)
Ne–Xe	.205	.260	.301	.300	.359	.370(b)

Experimental values are of (a) Grew *et al.* (1954) and (b) Grew (1947).

REMARKS

It will be seen that the agreement between the calculated and experimental values is very satisfactory except in the case of $A-Kr$. This may be due to some errors in the assumed values of the force parameters for Kr in the calculation of α_T. For A-Xe and Ne-Xe the agreement becomes poor at 185°K which seems to be due to Xe approaching its liquefaction point.

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Letters to the Editor

The Board of Editors will not hold itself responsible for opinions expressed in the letters published in this section. The notes containing reports of new work communicated for this section should not contain many figures and should not exceed 500 words in length. The contributions must reach the Assistant Editor not later than the 15th of the second month preceding that of the issue in which the letter is to appear. No proof will be sent to the authors.

3

ANISOTROPY OF WATER CLUSTER ABOUT THE Cu^{++} ION

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The ground state of Cu^{++} ion ($3d^9\ ^2D_{5/2}$) in octahedrally co-ordinated salts under the influence of the usual type of cubic crystalline electric field with positive coefficient (Van Vleck, 1932, Schlapp and Penney, 1932 and Gorter, 1942) splits into an orbital doublet and triplet above it.

Beevers and Lipson (1934) have shown that the water cluster about the Cu^{++} ion has the approximate tetragonal symmetry and hence according to the theories of Polder (1942), Abragram and Pryce (1951), Bleaney *et al.* (1955) and Bose *et al.* (1957) the ionic magnetic anisotropy of the Cu^{++} ion is given by

$$K_{\parallel} - K_{\perp} = \Delta K = \frac{2N\beta^2}{kT}(-\lambda + kT)\,.\,D' = \frac{2N\beta^2}{kT}\ (-\lambda + kT)\,.\,D.f^2$$

where $K_{\parallel}$ and $K_{\perp}$ are the ionic susceptibilities parallel and normal to the tetragonal axis respectively; $D = \left(\frac{4}{E_{\parallel}} - \frac{1}{E_{\perp}}\right)$, where $E_{\parallel}$ and $E_{\perp}$ are the energy differences of the lowest basic doublet and the two tetragonal levels respectively of the triplet; and f^2 is the covalency factor (Owen, 1955).

Our measurements of the absorption spectra of Cu^{++} ion in copper sulphate in aqueous solution at first sight show that there is only one band having maximum at 12,400 cm^{-1}, but a closer examination of the absorption curves (fig.1) shows that there is another maximum at about 12,000 cm^{-1}. The second maximum is directly noticeable, though it is not very prominent. There is a great deal of experimental evidences (Ballhaussen and Jorgensen, 1954) that the absorption

curves of cupric ion in aqueous solution in different amino copper complexes consist of at least two discernible bands.

If this separation is taken to be due to the tetragonal component of the crystal field then one can calculate D, which when substituted in the above expression will give $\Delta K/f^2$. Now according to Owen's findings and also of ours (Mookherji and Chhonkar, 1959) f^2 in $CuSO_4$ aqueous solution is 0.85 which gives directly ΔK in solution state for the water cluster about the Cu^{++} ion. Since we have found in our studies of nickel salts (Mookherji and Chhonkar, in course of publication) ΔK in state of solution and in crystalline state does not differ appreciably and hence our evaluated value of ΔK in case of $CuSO_4$ solution should agree with that of crystal value of ΔK (Bose *et al.* 1957) provided that our optical findings are correct. $\Delta K = 548.4 \times 10^{-6}$ at $300°K$ as obtained by Bose *et al* (1957) from magnetic studies agrees well with our calculated value of $\Delta K = 548 \times 10^{-6}$ at the same temperature and hence we conclude that the first and second maxima are due to tetragonal splitting.

Since our assignment agrees well with the magnetic findings we have calculated f^2 evaluating ΔK from our optical measurements and utilising Bose *et al.* (1957) magnetic ΔK —values. They are given in Table I. We find that f^2 —values are of the right order and almost the same for all the salts studied in agreement with the suggestions of Bose *et al.* (1957) for these salts.

TABLE I

Sulphate series					
Pentahydrate	K	NH_4	Rb	Ti	Zn–K
0.85	0.88	0.76	0.875	0.81	0.88
Selenate series					
Pentahydrate	K	NH_4			
0.865	0.88	0.83			

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4

APPLICATION OF SIGN RELATIONS IN THE CASE OF 4, 1, 3-CHLORO-DINITRO-BENZENE

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The method of systematic application of sign relations as developed and described by Grant, Howells and Rogers (1957) was tried for the sign determination of the structure factors of (*okl*) reflections from (4 : 1 : 3) chloro-dinitro-benzene and found to be very successful.

(4 : 1 : 3) chloro-dinitro-benzene (α-modification) belongs to orthorhombic space group Pccn D^{10}_{2h} with $a = 8.96$, $b = 11.08$, $c = 15.73$ Å and with eight molecules per unit cell [Gopalakrishna. (1959)]. The (100) projection is of pmg symmetry.

Of the 96 observed $|F(okl)|$'s, 40 with larger $|U|$ values were used in the process, which gave rise to 300 distinct triple sign relations of the type

$$S(h')S(h+h') \approx S(h)$$

and about 100 sign coincidences from different pairs of triple sing relations of the type

$$S(A)\ S(B)\ S(C_1) \approx +1$$
$$S(A)\ S(B)\ S(C_2) \approx +1$$

The signs of seven structure factors (of k = even, l = even) were obtained from the sign relation of the type

$$S(o, 2k, 2l) \approx S(okl)\ S(o\bar{k}\bar{l}) = +1$$
$$S(o, 2k, o) \approx S(okl)\ S(ok\bar{l}) = (-1)^k$$
and $$S(o, o, 2l) \approx S(okl)\ S(o\bar{k}l) = (-1)^k$$

Starting with the signs of these seven structure factors and using the sign coincidences, all the forty terms were assigned signs. The iterative process corrected 13 signs out of those 40 after four cycles of the process, when all the signs were consistent with each other. The electron density map calculated with these forty factors gave out the position of chlorine atom and the approximate orientation of the molecule. Later, the signs of another 15 terms were determined from the triple sign relations. When the contribution due to these fifteen terms was added to the previous map, the approximate positions of all the atoms became

evident. Using these positions and calculating the structure factors, the R-value was about 0.40. Fig. 1 shows the electron density synthesised with 90 terms. When the structure factors were calculated using the atomic co-ordinates from this figure, only one was found to be not correct among the previously determined 55 signs.

The $|U|$ values were calculated from intensities measured by visual comparison and were on an arbitrary scale. They were not corrected for absorption nor for temperature effect.

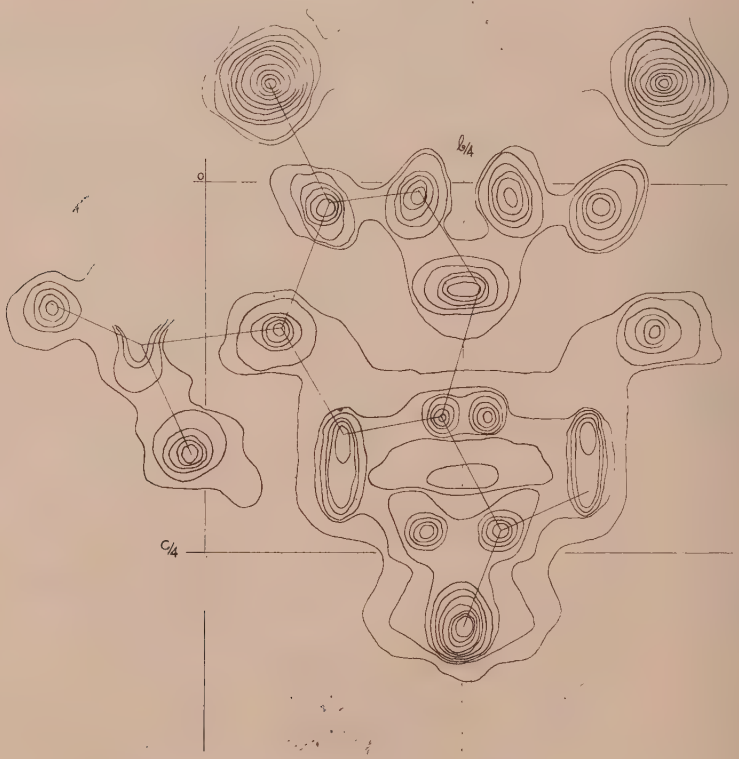

Fig. 1. Electron density map (100) projection calculated with 90 terms.

The results obtained in this case show that the method under favourable conditions yields a tentative solution even without any previous knowledge of the stereo chemistry of the molecule or of any signs of the structure factors. The presence of the chlorine atom among the lighter ones does not prevent the method from yielding a solution. The random and systematic errors in $|U|$ values do not seriously affect the sign determination by this method.

TABLE I

y and z co-ordinates of atoms (without refinement)

	y/a	z/c		y/a	z/c
Cl	.063	−.070	C	.208	.007
C	.117	.017	N	.263	.233
C	.067	.103	O	.250	.300
			O	.371	.210
C	.133	.175	N	−.054	.113
C	.229	.163	O	−.017	.183
C	.241	.075	O	−.154	.068

The complete structure analysis after refinement will be published later.

The author wishes to express his deep indebtedness to Prof. B. N. Srivastava, D.Sc., F.N.I., for his keen interest and valuable discussions. He expresses his gratefulness to Dr. B. V. R. Murty for suggesting this work and guiding.

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REVIEW

RUSSIAN-ENGLISH GLOSSARY OF ACOUSTICS AND ULTRASONICS. Pp. 170+xxiii. Consultant Bureau Inc. 227 West 17th Street, New York, N.Y. 1958. Price 10.00.

This volume gives the English-equivalents of all the words and phrases which are expected to be found in the literature dealing with topics on acoustics and ultrasonics. The words in Russian are written in Russian alphabet. Many of words and phrases are also found in the literature dealing with topics on other branches of physics. An index of Russian-equivalents of names of all the authors who have published papers in acoustics and ultrasonics has also been included.

It is needless to mention that the glossary will be extremely helpful to the workers who want to translate papers on these topics published in Russian journals. The volume is not bound, but the printing paper used is of high quality.

S. C. S.

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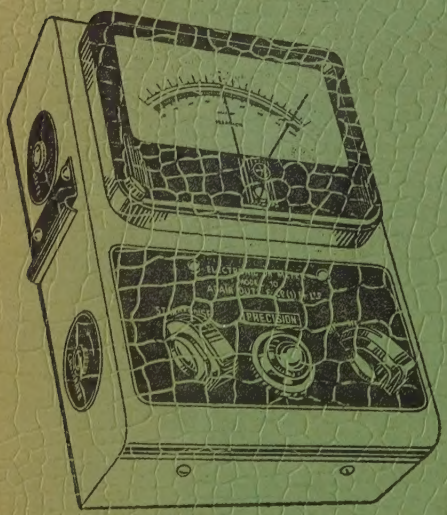

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